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Icarus: A 2-D Direct Simulation Monte Carlo (DSMC) Code for Multi-Processor Computers

User's Manual - v 10.0

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Icarus: A 2-D Direct Simulation Monte Carlo (DSMC) Code for Multi-Processor Computers

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ABSTRACT

Icarus is a 2D Direct Simulation Monte Carlo (DSMC) code which has been optimized for the parallel computing environment. The code is based on the DSMC method of Bird[11.1] and models from free-molecular to continuum flowfields in either cartesian (x, y) or axisymmetric (z, r) coordinates. Computational particles, representing a given number of molecules or atoms, are tracked as they have collisions with other particles or surfaces. Multiple species, internal energy modes (rotation and vibration), chemistry, and ion transport are modelled. A new trace species methodology for collisions and chemistry is used to obtain statistics for small species concentrations. Gas phase chemistry is modelled using steric factors derived from Arrhenius reaction rates or in a manner similar to contiuum modelling. Surface chemistry is modelled with surface reaction probabilities; an optional site density, energy dependent, coverage model is included. Electrons are modelled by either a local charge neutrality assumption or as discrete simulational particles. Ion chemistry is modelled with electron impact chemistry rates and charge exchange reactions. Coulomb collision cross-sections are used instead of Variable Hard Sphere values for ion-ion interactions. The electro-static fields can either be: externally input, a Langmuir-Tonks model or from a Green's Function (Boundary Element) based Poison Solver. Icarus has been used for subsonic to hypersonic, chemically reacting, and plasma flows.

The Icarus software package includes the grid generation, parallel processor decomposition, post-processing, and restart software. The commercial graphics package, Tecplot, is used for graphics display. All of the software packages are written in standard Fortran.

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A PDF version of this manual (with color images) is available for downloading; please contact the first author for more information. PDF versions of the papers in section 12 are also available for downloading. Please contact the first author about availability of the code.

Table of Contents

1.0 Direct Simulation Monte Carlo (DSMC): Background

1.1 Method

DSMC is a method for the direct simulation of rarefied gas flows[11.1]. The method assumes that the gas is a dilute gas; that is, binary collisions dominate the molecular interactions. The flow domain is first divided into a number of cells. The cell size is determined by the local mean free path, λ,; a cell size ~ $\lambda/3$ is typically recommended. Unlike CFD grids with mesh orthogonality and one-to-one cell side correspondence constraints, the DSMC grid system serves only to identify a volume for choosing collision partners and for obtaining sampling statistics. The flow field is simulated using a number of computational particles (some 10^7particles are not atypical for runs on massively parallel supercomputers). Particles consist of all kinds of species such as radicals, ions, and molecules. The species type, spatial coordinates, velocity components, internal energy partitioning, and weight factor of each computational particle are stored. As the particles move through the domain, they collide with one another and with surfaces. New particles may be added at specified inlet port locations, and particles may be removed from the simulation due to chemical reactions or through the pumping ports. Since this is a statistical method in which the system evolves in a time-like manner, a steady-state solution is then an ensemble average of a number of solution time steps (snapshots of the system) after the flow field has reached a steady-state. *Icarus* can also be run in a *time accurate mode* to model unsteady problems.

The basic premise of DSMC is that the motion of simulated particles can be decoupled from their collisions over a time step. The size of the time step is selected to be a small fraction of the mean collision time, or a fraction of the transit time of a molecule through a cell (similar to an explicit CFL constraint). During the motion phase, particles move in free molecular motion according to their starting velocity and any body forces acting on the particles (for example the Lorentz force on charged species). During this phase, particles may cross cell boundaries, collide with walls and undergo surface chemistry, or exit the flow field. During the collision phase, random collision pairs are selected from within each cell *regardless of the position* of the particles within the cell. The no-time-counter (NTC) technique [11.3], is used to determine the computational particle collision frequency. The number of pairs to be selected from a given cell at a time step is

$$\text{\# pairs} = 1/2\ N\ \overline{N}\ F_n\ (\sigma_T C_r)_{max}\ \Delta t\ /\ V$$

where N is the number of computational particles in the cell, F_n the number of real particles per simulated one, $(\sigma_T C_r)_{max}$ is the maximum of the product of the total cross-section and relative velocity for the pairs in the cell and V the cell volume. The pair collision is then computed with a probability $(\sigma_T C_r) / (\sigma_T C_r)_{max}$. This technique does not have the disadvantages of the older time counter (TC) method while maintaining computational efficiency, i.e., the simulation time is proportional to the number of molecules. This is a great advantage of DSMC as compared to other particle simulation methods such as molecular dynamics. Also, the NTC method allows for unsteady flows to be simulated in a time accurate manner. A collision limiter model is used to improve computational performance at high pressures. The model simply limits the number of collisions in a cell to a multiple of the number of actual collisions. This model has been shown to reproduce inviscid flow fields and has been used to model high pressure (2 atm) nozzle expansions into a vacuum.

Although only two position coordinates (r, z) of each simulated particle are stored, collisions are handled as three dimensional events to correctly conserve momentum transfer. The molecular model used for collision cross sections is the variable hard sphere (VHS) model [11.1]. According to this model, the collision cross section σ_{ij} depends on the relative speed (energy) of the colliding partners E_c as

$$\sigma_{ij} = A_{ij} E_c^{-\omega}$$

where A_{ij} is a constant and $\omega = s - 0.5$, with s the exponent of the dependence of the coefficient of viscosity on temperature. The chief advantage of the VHS model is that, although the collision diameter is allowed to vary with the relative speed (unlike the constant cross section hard sphere model), when a collision does occur, the post-collision velocity components are computed as if it were a hard sphere collision; that is, isotropic scattering in the center of mass frame of reference.

The DSMC technique can easily model internal energy modes: rotational and vibrational energies. The phenomenological Borgnakke and Larsen [11.2] model is used to determine the post-collision internal energy partitioning given the number of internal degrees of freedom of each species. This is a harmonic oscillator model which drives the post-collision energy distribution towards equilibrium. Recently, Marriott[11.5] and Gallis[11.6] has applied the Maximum Entropy strategy for particle systems to obtain this energy distribution; unfortunately, the complex chemical species in typical manufacturing plasma etch systems are poorly characterized so typically only translational nonequilibrium is modelled. Both models are included in the code.

Gas phase chemistry consists of six models: elastic gas reaction, charge exchange with functional cross-section fit, charge exchange using the model of Rapp and Frances, electron impact reactions for ionization or neutralization reactions, Arrhenius equation based continuum reaction modelling and inelastic electron impact reactions for the electron energy equation. Elastic collision gas phase chemistry is modelled using steric factors derived from Arrhenius reaction rates. That is, the chemical reaction probability given a particle collision is determined assuming a local Maxwellian distribution to convert the rate to a energy dependent probability. Charge exchange reactions model the exchange of both energy and momentum between neutral and charged species. Electron chemistry models electron impact chemistry using energy dependent rates and local electron number density and temperature. These rates are converted into a total reaction probability. That is, a probability which includes both collision and reaction rates. Surface chemistry is modelled with surface reaction probabilities; a optional, energy dependent, site coverage dependent model can also be used. The grid generation/preprocessor code, init2d, will input gas phase chemistry input in either a simple asci format or the standard CHEMKIN format.

1.2 Grid Characteristics

Icarus uses a multi-block system of algebraic meshes to define the computational domain. The grid is generated using the input processor program, *init2d*. This simple grid system allows great flexibility for capturing local high gradient regions without excessively griding the entire domain because there is no requirement for side correspondence between regions. See the paper by Bartel and Plimpton in Section 12.1 for more details.

As mentioned before, the key assumption in DSMC is that particle transport is de-coupled from particle-particle interaction. Therefore particles move without collisions for a specified time step, and then collision partners are chosen probabilistically from within a defined grid cell. Implementation of this method requires that the cell sizes and the time step be chosen carefully; particles should not travel longer than the mean free path(λ) in a time step and the unit cell should be sized approximately less than λ. The Knudsen number (Kn) and the Courant number (CFL) are quality metrics for the cell size and the time step:

(Kn > 1) = λ / cell length

(CFL < 1) = particle velocity / (cell length / time step)

The cell Kn and CFL numbers are output from the DSMC code in the *cell.** file and are used to verify that the particle transport assumptions were obtained.

1.3 Cell and Species Weighting

Icarus uses several strategies to obtain sufficient statistics for both local regions of disparate densities and for 'trace' species which have a very small mole fraction. First, each grid cell has a 'weight' which is simply used to spatially adjust the global or input ratio of real-to-computational particles. This 'cell weight' is initially proportional to the cell volume; this results in an equal number of computational particles per cell for a uniform initial density. As the simulation progresses, the number of particles in a given cell can become extremely large due to either chemical events or mass injection into the system. The 'cell adaption' logic of Icarus dynamically 'adjusts' the cell weight to maintain an upper bound on the number of computational particles per cell. Thus the user can be assured of sufficient statistics without a few cells with an unreasonable number of particles. This feature is transparent to the user.

Species weighting is another method which is used to increase the sampling statistics for the simulation. In this strategy, species which occur in small, trace amounts have a lower 'computational worth' than do other species. For example, in low density plasma systems, the ionization fraction is very small: < 0.1%. Thus, the neutral species will have a single weight of 10^{10} molecules or atoms per computational particle while the ions which occur in trace amounts will have a weight of 10^6 ions per computational particle. The code is limited to two species weight multipliers: 1.0 for the base or full case and a number less than 1.0 for all the trace species.

1.4 Elastic Scattering Cross Section

The Variable Hard Sphere (VHS) model treats each molecule as a fixed diameter sphere with isotropic scattering. The VHS model employs the simple isotropic scattering law of the hard sphere model but accounts for the temperature dependence of the collision cross section by use of a single parameter which may be determined from the viscosity temperature dependence

$$\sigma = \sigma_{ref}\left(\frac{T}{T_{ref}}\right)^{-\omega}$$

where σ_{ref} is the collision cross section at the reference temperature, T_{ref}, and T is the kinetic temperature of the collision partners. The VHS parameter, ω is related to the temperature exponent of viscosity, s

$$\eta = \eta_o\left(\frac{T}{T_o}\right)^{s}$$

as $s = \omega + \frac{1}{2}$; where η is the viscosity and subscript o denotes the reference temperature and viscosity (see ref. [11.1])

A database of viscosity index, ω, and molecular diameters at the reference temperature for approximately 150 species has been compiled and given in Chapter 10.2. Curve fits to viscosity of species not listed can be used to obtain s (the slope) and therefore ω.

Icarus contains a method to extend the computationally efficient pressure range to higher pressures. A collision limiter model is used: the number of computational collisions per computational particle in a time step is constrained. This method has been shown to reproduce inviscid flow systems. The enclosed AIAA paper by Bartel, Sterk, Payne, et.al. (Section 12.3) contains the details and method comparisons.

1.5 Internal Energy Exchange

In a typical application the particle simulators may possess internal degrees of freedom, rotational, vibrational and electronic. The most common application is that of a particle with 2 rotational and 2 vibrational degrees of freedom, such as oxygen and nitrogen molecules. One way to deal with internal energy exchange is to define cross sections for all the possible allowable transitions. However, for most cases the number of states that needs to be included is so large that this approach is not practical. In DSMC the model that has been almost universally used since its introduction on 1974 is the phenomenological model of Borgnakke and Larsen (see Bird chapter 5 [11.1]) and its variants. According to this model the relaxation process is modeled by assuming that only a fraction of the collisions is inelastic.

The particular Borgnakke and Larsen method used in Icarus is the serial application of the method. According to this, energy is partitioned in a serial fashion, starting with any mode and distributing energy between that mode and an energy pool that contains all the undistributed collision energy. For more details about the method the reader is referred to Bird's monograph[11.1]. Icarus offers the option of treating the vibrational mode in a quantized mode following the harmonic oscillator model. The parameters for the harmonic oscillator model for some gases are giv-

en in Appendix 1 of Bird's monograph[11.1]. The relaxation parameters can be defined to be either constant or a function of the total collision energy ("*collision temperature*"). Since there is no universally accepted model for the relaxation rate, for the particular case of nitrogen flow Icarus offers the option of a temperature dependent relaxation rate. In the general case this is to be considered as a place holder and if gases other than nitrogen need to be simulated the appropriate relaxation rates need to be added to the code.

1.6 BGK

Icarus incorporates a method to perform collisions in a collective manner. The method is based on a simplified version of the Boltzmann equation the BGK method. The application and adaptation of the BGK method to DSMC is detailed in AIAA 2000-2360 (Section 12.10), where it was found to be in good agreement with the standard DSMC collision algorithm. It should be noted that currently the method is only applicable to monatomic gases. Future extensions of the method will include the internal degrees of freedom.

1.7 Plasma Features

Icarus contains several additional models for the simulation of ionized gases. First, the electrons can be considered to be in local charge neutrality (LCN) with the ions (usually valid when the Debye Length is much smaller than a characteristic cell length) or can be modelled as discrete particles in a similar fashion as a PIC plasma code. The LCN assumption can generally be used in geometries where the sheath is much smaller than the overall domain of interest. In this case, the electron number density is simply the sum of the ion charge density. Unlike other DSMC LCN investigators, we simply define a local electron number density, n_e, in a manner consistent with continuum formulations. We assume that the electrons have a Maxwellian distribution and use a continuum formulation with Arrhenius rates to compute any electron chemistry; we include reactions for ionization, neutralization, and inelastic scattering. We have found that this yields much better results than trying to use pseudo-electron particle chemistry.

There are three options to determine the electron temperature, T_e: use a constant value, use a control volume formulation which includes power deposition, and a kinetic model which periodically generates electron kinetic particles solely for the purpose of determining the Te. In the latter option, cross-sections are used for the chemistry since a distribution function is not assumed. A fourth option is included which maintains a constant product of neTe for each cell; this strategy essentially assumes a constant electron energy in a cell and when the electron density increases, its mean temperature must decrease and *vice versa*.

The electro-static fields can be assumed to be ambipolar and a standard Langmuir-Tonks formulation used or a Poisson equation is directly solved using a Boundary Element Method [11.7]. Obviously the first treatment is computationally much faster than the second and also tends to smooth out dynamic or statistical fluctuations. In the ambipolar method, the gradient of

neTe is obtained by using linear quadrilateral shape functions (setup automatically in init2d); a time averaged value for ne is used to reduce statistical noise. In the Poisson approach, the standard equation for the electro-static potential is solved in either cartesian or axisymmetric coordinates.

$$\nabla^2 \varnothing = \rho / \varepsilon_o$$

where ρ is the charge density and ε_o is the permittivity of free space. The electro-static fields are determined from the gradient of the potential

$$E_x = -\frac{\partial \varnothing}{\partial x}$$

$$E_y = -\frac{\partial \varnothing}{\partial y}$$

Again the linearized shape functions are used to determine the gradients. A BEM strategy is used since the multi-block grid format does not require region-to-region direct cell side association and therefore a traditional FV or FD method would have to consider the region interfacial cells as a special case. However, the BEM method solves for the potential using volume integrals; one should note the new option for defining surface elements where multiple elements can be associated with a surface cell. This option was a direct consequence of using BEM and will increase the accuracy of its solution without simply increasing the cells which greatly increases the computational time.

Several options exist in an attempt to smooth or filter the fluctuating cell charge density. These inherently assume that the electron plasma frequency is not a dominate effect and that the ion and neutral effects are of interest. However, one can always choose the PIC mode where the charge density is the instantaneous value so that the electron frequency can be resolved. The traditional DSMC-like charge averaging method, where the charge is taken as the average of the sample before it is zeroed during the unsteady phase, can be used; however, it can introduce non-physical oscillations when the sample size is reset. A true sliding average method has been included which *slides* the sample size in time. This has been shown to greatly reduce the non-physical fluctuations. For both methods, the charge density to be used in the Poisson solver can be backward time averaged by a simple user defined weight factor.

1.8 Code Validation

Icarus has been validated over a wide range of problems. The papers in Section 12 contain some of these. The pressure range has varied from very low pressure applications of space orbital conditions which are free-molecular flow to two atmosphere pressure systems which are highly collisional. The problems have also varied from non-reacting to chemically reacting with internal degrees of freedom. Recent work has included electro-static forces for plasma problems.

1.9 Computer Platforms

Icarus is a 2-D DSMC code which can model systems in either cartesian or axisymmetric coordinate systems. This code was written to take advantage of distributed memory parallel computer systems; either massively parallel system or workstations with a few processors. The message passing calls are written in MPI. MPI libraries are freely available for UNIX platforms (see the WWW); commercially available options exist for MS-NT/2000 mp systems. The enclosed AIAA paper by Bartel and Plimpton in Section 12.1 describes the basic strategy used for the parallel method. This strategy is directly extendable to 3D and allows timely computation of large problems which were previously unsolvable. Although the code was written to take advantage of multi-processor systems, it can also be executed on single processor workstations or PCs.

1.10 Source Code Control

The first author (Bartel) maintains Icarus under source code control using the Component Software RCS system for Windows.

2.0 Overall Code Structure

The **Icarus** code requires pre- and post-processor programs. Table 1 is a summary of the individual program names, program descriptions, and the files that each program uses and creates. Throughout this manual, program names are indicated by bold type and file names are identified by italics.

Table 1: DSMC 2D Code Descriptions

Code	Description	Input Files	Output Files
init2d	Grid generation and problem description. Converts geometry and chemistry information to **icarus** format.	*geometry.inp, <spec>, <inlet>, <surf_bc>, <chem>,<chem.asc>, <cross_section>*	*<datap>, <grid>,<init2dout>*
decomp2d	Decomposes problem for parallel environment. This code is not necessary for single processor use.	*<datap>*	*dsmc.node, dsmc.in2*
icarus	Performs DSMC calculation and gathers statistics. Typically run in parallel environment.	*dsmc.in, dsmc.in2(MP), datap(1P), <dsmc.restart>,*	*cell.*, surf.*, wafer.*, chem.*, plasma.*, particle.*, dsmc.log, dsmc.pump*
restart2d	Converts previous DSMC simulations with same grid for a starting solution for a new calculation.	*cell.*, dsmc.in2, dsmc.node*	*dsmc.restart*
regrid2d	Interpolates from a different grid to a new grid to produce a starting solution	*cell.*, dsmc.in2, dsmc.node, btecplot*	*dsmc.restart*
post2d	Converts cell information (particle statistics) to macroscopic quantities(i.e., pressure, density, species concentrations, velocities, etc.)	*cell.*, (or chem.*, plasma.*) post2d.vlist, datap*	*cellout*
surface2d	Converts surface element information to incident flux, reflected flux (etchant), surface coverage, surface pressure, shear stress and heat flux.	*surf.*, datap*	*surfout*
waferxy2d	Converts wafer information to angular and energy distribution of incident particles by species. Only for material specified as a wafer in *geometry.inp*.	*wafer.*, datap*	*waferout*
stat2d	Determines convergence between two different **icarus** *cell.** files.	*cell.*, cell.***	*stat.out, stat.tec*

3.0 init2d - Icarus Preprocessor Program Description

3.1 Overview

In this section, the input files for the preprocessor **init2d** will be presented. This program converts the geometry, chemistry and DSMC parameters input by the user, into the format required by **icarus**. All input is in MKS units. All the file names can be user defined. The files used in **init2d** contain the following information:

geometry.inp	Grid information and DSMC parameters (file name is determined by user, but typically has *.inp extension.)
spec	Chemical species information.
chem	Gas phase reactions, rate constants and heat of reaction.
chem.asc	Gas phase reactions chemistry information using alternate Chemkin format in place of the standard Icarus *chem* file.
surfbc	Surface boundary conditions: chemical reactions, reaction probabilities, creation probabilities, permeability, and boundary conditions for electro-static fields.
inlet	Specifies flowrate and location for gas injection into the domain; a point source injection, an outgassing surface, and freestream inflow are examples of inlet options.
cross_section	Input collision cross sections used instead of the variable hard sphere(VHS) elastic interaction model or chemical reaction cross sections.

3.2 init2d Code Description

Goal: -generate a graphical file to display grid
-generate an input file for the **icarus** code

Usage: **init2d** *geometry.inp*

Input files:

geometry.inp: input data file for problem definition: grid, boundary conditions, etc.

the following filenames are defined in geometry.inp:

spec - species definition file

chem - gas phase chemistry input optional

chem.asc - Chemkin format gas phase chemistry format
surf_bc - surface boundary condition input
inlet - inlet boundary file
cross_section - elastic & chemical cross sections

Output files:

filenames are defined in the geometry.inp file

datap - input file for **icarus** or **decomp2d**
grid - Tecplot formatted file of grid description
init2d.out - echo of last portion of the screen output

3.3 Grid Characteristics

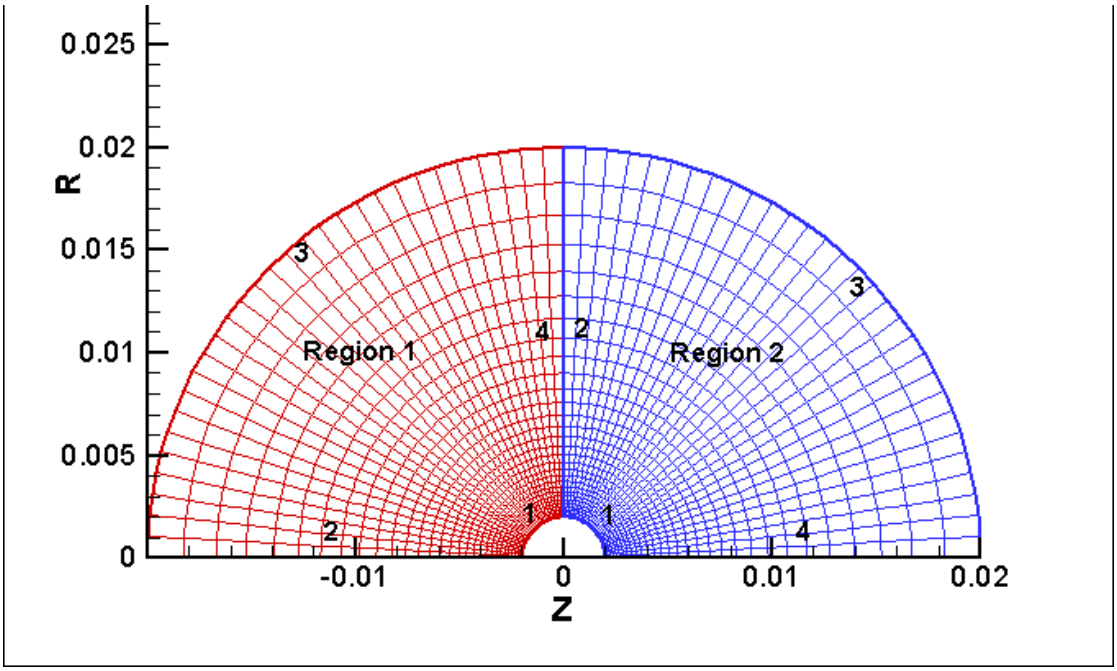
See the papers in Appendix A for examples of the multi-blocked algebraic grid strategy which is used in **init2d**. Also, numerous examples are found in Appendix B. The user has complete freedom in placing the grid blocks; cell side correspondence between blocks is not a requirement. The user should be warned that the choice of grid structure can effect the results since the basic premise of the DSMC method is that collision pairs are chosen probabilistically within a cell and thus the cell size should be < mean free path. For example, simulation of expanding flows (see the NO expansion example in Chapter 11) require care to determine the correct collision frequency when the flow is essentially a spherical expansion. In summary, the order of the regions is not important (e.g. region can be connected to region 99); however, the regions must be sequential starting with region 1.

3.4 Input File Description (geometry.inp)

The input file is split into 3 logical blocks:

1) the input options block
2) the basic grid block definition with corner point definition
3) detailed description of each grid block and flow connectivity.

An example geometry.inp file for a flow over a 1/2 sphere is shown. This problem consists of regions or blocks; the flow is from left to right. Although the interface cells between region 1 and 2 are in 1-to-1 correspondence, it is not a requirement of this code.



From the 'sphere' test case, sphere2.inp is shown with the three sections indicated:

First Section

```
*-------------------------------------------------------------------------
*   asterick in column 1 indicates comment card
*-------------------------------------------------------------------------
*
 ICF target sphere
*
*
*-------------------------------------------------------------------------
*
control    1      -1 -- plot grid only;
*                  1 -- initialization & plot file
*
type       1              0/1 for X-Y or Z-R flow
*
```

Second Section

```
*
read general grid
*-------------------------------------------------------------------
*                    Region Definition
*-------------------------------------------------------------------
     2          number of regions (must be .le. 30)
     6          number of global points (must be .le.120)
*--------------------------------------
```

```
*     Global corner pt. coordinates
*  Pt.       z (m)          r(m)
*---------------------------------------
1  -0.02    0.
2  -0.002    0.0
3   0.002    0.0
4   0.02   0.0
5   0.0    0.002
6   0.0    0.02
*
```

Third Section

```
*-----------------------------------------------------------------------
*            Individual Region Definitions Follow
*            --REGION NUMBERS MUST BE SEQUENTIAL--
*-----------------------------------------------------------------------
*=======================================================================
region   1  <------  Inputs specific to this region follow
*=======================================================================
grid
   2             global points
   1
   6
   5
   30          number of cells along sides 1 and 3
   30            number of cells along sides 2 and 4
   1             sides 1 and 3 curvature: 0/1 for line/circular arc
   0             sides 1 and 3 cell spacing:
   2  1.1   150.            sides 2 and 4 cell spacing:
   5             boundary type code for sides 1 - 4, resp.
   1
   3
   7
   3
*-----------------------------------------------------------------------
*   Side  Cell1  Cell2   elem/cell  Spec. refl.   Temp. K    Material#    Value
*-----------------------------------------------------------------------
    1     1     5       1            0.000       18.00        0          0.
    1     6     15      3            0.000       18.00        0          0.
    1     16    500     1            0.000       18.00        0          0.
*-----------------------------------------------------------------------
*                 Region interface/matching
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*-----------------------------------------------------------------------
       1          0
       2          0
       3          0
       4          1           2    2
*=======================================================================
*=======================================================================
```

```
region   2  <------  Inputs specific to this region follow
*=====================================================================
grid
   5            global points
   6
   4
   3
   30          number of cells along sides 1 and 3
   30            number of cells along sides 2 and 4
   1             sides 1 and 3 curvature: 0/1 for line/circular arc
   0             sides 1 and 3 cell spacing:
   2  1.1   150.            sides 2 and 4 cell spacing:
   5             boundary type code for sides 1 - 4, resp.
   7
   3
   1
   1
*---------------------------------------------------------------------
*   Side  Cell1  Cell2   elem/cell  Spec. refl.   Temp. K    Material#    Value
*---------------------------------------------------------------------
    1     1     500       1          0.000       18.00        0          0.
*---------------------------------------------------------------------
*                  Region interface/matching
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*---------------------------------------------------------------------
       1          0
       2          1        4    1
       3          0
       4          0
*=====================================================================
*=====================================================================
*---------------------------------------------------------------------
END                  END OF EXPERT INPUT FILE
*---------------------------------------------------------------------
```

An asterisk, *, or # in column 1 indicates a comment card--blank lines are not allowed. An **i** indicates an integer input and a **r** indicates a real number input. Each section can contain optional key word entries.

Section 1:

Example:

```
*-----------------------------------------------------------------------
*   asterick in column 1 indicates comment card
*-----------------------------------------------------------------------
*
 ICF target sphere
*
*
*-----------------------------------------------------------------------
*
control    1      -1 -- plot grid only;
*                  1 -- initialization & plot file
*
type       1              0/1 for X-Y or Z-R flow
*
```

First data entry MUST be a title.

optional key word entries:

control **i**

-1	obtain grid file only -- useful for initial stages of grid generation
1	full mesh and problem initialization (*default*)
2	full mesh and problem initialization with debug output
3	read a Tecplot formatted save file from a Navier-Stokes simulation to check initial grid spacing.
4	read an dsmc file from post2d to check initial grid spacing.

type **i**

0	cartesian x-y (*default*) **(Note, Y must be >= 0.0, depth of 1 meter is assumed.)**
1	axisymmetric z-r **(Note, Z is the first coordinate and R the second)**

debug flag **i**

0	no debug output (*default*)
1	debug output

base number ratio r

base number of real molecules per simulation one. This is one method to set problem size. See 'number per cell' option for the preferred method.

1.e10 (*default*)

number per cell r

this determines the number of real molecules per simulation one to obtain this minimum number per cell for an initial density distribution (see inlet file).

20 (*default*)

particle flag i

determines how the simulation particle representation will be determined:

0 use minimum number per cell (*default*)

1 use base number ratio

base dt r

base time step for particle move and collision. this can be modified in the Icarus input file.

1.e-6 (*default*)

cell weight i

this sets various cell weighting strategies. These are very problem specific; see the examples section for various applications.

Cell Weighting options:

0 region number and dt based on base number and base dt with a input region ratio (definition of base number and dt refer to variables 13 and 14)

1 local cell weights based on volume, region dt from base dt and region ratio

2 local cell weights based on volume and option 0

3 local cell weights based on volume, region ratio, and region dt base value (constant dt for all cells)

4 local cell weights based on volume and region ratio, with region dt based on base value of dt (*default*)

-2 uses option 2 with radial expansion assumption from origin. This varies the cell weights in a $1/r^2$ manner--typically used for nozzle exit flow expansions.

```
x > 0.0
r > rmin
wt = wt / (r/rmin**2)
```

-3 similar to option 3 but with radial expansion model

-4 similar to option 4 but with radial expansion model

thermal acc. r

the wall thermal accommodation coefficient. This can decouple the momentum and energy accommodation at the walls

1.0 (*default)*

pump region i

specify the region for the pump model to apply. This model will probabilistically delete particles in a given region to maintain a given pressure at a location. This model is for a volume displacement pump such as a turbo-molecular pump.

wafer surface i

specify the surface material number of obtain incident particle angular and energy distributions for each species. The use of this option increases the memory requirements since detailed binning is required for each surface element with this material type.

expansion radius wt r

one of the cell weight models assumes a radial expansion. This input is the nozzle radius. The radial expansion model is not applied to cells within this radius. The nozzle exit plane is assumed to be at z = 0.0.

1.e-6 *(default - m*)

radial wt factor r

the radius below which the cell weights are set to 1.0 (this is not commonly used)

0.0 (*default*)

gravity flag i

the sign of the gravity vector (assume 1 m/s-s).

0.0 (*default*)

1. or -1. (option)

read cross_section i

flag to read a file which can contain fits to the elastic cross sections or chemistry reactions. see cross_section file input for file name.

0 do not read (*default*)

1 read file

overwrite files i

by default, init2d will not overwrite the output files (datap & grid). This option overwrides this check.

0 off (*default)*

1 on

plasma option i

flag to add additional data to the output file (datap). Use this option when plasmas (poisson solutions) are to be required in the simulation.

0 do not use (*default*)

1 use

species file filename
spec (*default)*

inlet file filename
inlet *(default)*

surface file filename
surfbc *(default)*

chemistry file filename
chem (*default)*

chemkin file filename
chemkin formatted chemistry file
chemkin_chem *(default)*

cross_section file filename
crossection *(default)*

output data file filename
datap *(default)*

grid file filename
grid *(default)*

output file filename
the echo of the last portion of the screen output from the init2d setup.
init2d.out *(default)*

eps file filename
the plasma permittivity (8.854e-12 (F/m). this option is not implemented at the current time.
plasmaeps *(default)*

Section 2:

An asterisk, *, or # in column 1 indicates a comment card--blank lines are not allowed. An **i** indicates an integer input and a **r** indicates a real number input. Each section can contain optional key word entries.

Example:

```
*
read general grid
*-------------------------------------------------------------------
*                  Region Definition
*-------------------------------------------------------------------
    2          number of regions (must be .le. 30)
    6          number of global points (must be .le.120)
*--------------------------------------
*    Global corner pt. coordinates
*  Pt.       z (m)         r(m)
*--------------------------------------
1  -0.02    0.
2  -0.002    0.0
3   0.002    0.0
4   0.02   0.0
5   0.0    0.002
6   0.0    0.02
```

read general grid

first item: The total number of regions in the DSMC grid. The regions are specified by four global corner points. Each region contains four sides with each side usually having a single specified boundary condition.

second item: Total number of global points. Not all global points must be used; extra values are allowed and order is NOT important.

third item (list): Global point definition given by global point number, and coordinates in meters.

NOTE: either Y (cartesian) or R (axisymmetric) MUST be > 0.0

for coordinate system X, Y (type 0):for coordinate system Z, R (type 1):
point #, x, y or point #, z, r

read test points

first item: The number of points to use in Icarus to specify the physical locations for pressure feedback in the pressure control pump model(s), the locations where velocity distribution function information can be obtained, or simply points where the pressure is obtained during the unsteady/steady portion of the simulation to aid in verifying steady-state flow behavior. The pump model allows pump speed (that is, volume deletion of particles) to vary to achieve a desired pressure at a specified point. The starting pump speed, pump speed limits, and desired pressure are specified in the Icarus input file. The velocity distribution function option will be described in the input section for Icarus.

if first item > 0: enter a list of *first item* values in the following format:
pump region number, (x or z value), (y or r value)
if first item < 0: enter a list of *first item* values in the following format:
pump region number, corner pt. number

Do not use a region global point or specify a point exactly on the perimeter; computer round-off may be a problem.

examples:

```
read test points    2
    1        1.0     1.5
    2        1.0     2.5
```

or

```
read test points    -2
    1   34
   2    24
```

Section 3:

Example:

```
*=====================================================================
region   1  <------  Inputs specific to this region follow
*=====================================================================
grid
   2            global points
   1
   6
   5
   30          number of cells along sides 1 and 3
   30            number of cells along sides 2 and 4
   1             sides 1 and 3 curvature: 0/1 for line/circular arc
   0             sides 1 and 3 cell spacing:
   2  1.1   150.            sides 2 and 4 cell spacing:
   5             boundary type code for sides 1 - 4, resp.
   1
   3
   7
   3
*---------------------------------------------------------------------
*   Side  Cell1  Cell2   elem/cell  Spec. refl.   Temp. K    Material#    Value
*---------------------------------------------------------------------
    1     1     5       1            0.000       18.00        0           0.
    1     6     15      3            0.000       18.00        0           0.
    1     16    500     1            0.000       18.00        0           0.
*---------------------------------------------------------------------
*                Region interface/matching
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*---------------------------------------------------------------------
       1          0
       2          0
       3          0
       4          1            2    2
*=====================================================================
region   2  <------  Inputs specific to this region follow
*=====================================================================
grid
   5            global points
   6
   4
   3
   30          number of cells along sides 1 and 3
   30            number of cells along sides 2 and 4
   1             sides 1 and 3 curvature: 0/1 for line/circular arc
   0             sides 1 and 3 cell spacing:
   2  1.1   150.            sides 2 and 4 cell spacing:
   5             boundary type code for sides 1 - 4, resp.
   7
   3
   1
   1
*---------------------------------------------------------------------
*   Side  Cell1  Cell2   elem/cell  Spec. refl.   Temp. K    Material#    Value
*---------------------------------------------------------------------
    1     1     500     1            0.000       18.00        0           0.
*---------------------------------------------------------------------
*                Region interface/matching
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*---------------------------------------------------------------------
       1          0
       2          1          4    1
       3          0
       4          0
*---------------------------------------------------------------------
END                 END OF EXPERT INPUT FILE
*---------------------------------------------------------------------
```

Each region block consists of the following format. An asterisk, *, or # in column 1 indicates a comment card--blank lines are not allowed. An **i** indicates an integer input and a **r** indicates a real number input.

region nr where nr is the region number. The regions must be entered in consequent, ascending order.

the following are optional commands:

fnum multiplier r

this multiplies the ratio of real/computational particle for this region
1.0 (default)

dt multiplier r

this multiplies the region time step
1.0 (default)

ic density multiplier r

multiplies the initial density of this region
1.0 (default)

ic density r

overrides the initial density from the inlet file for this region
default is density from inlet file

ic species fractions r_i, r_j, r_k, ... r_n

overrides the initial species fractions from the inlet file for this region
default is the fractions for the inlet file
input is one fraction per species per line

ic trans. temps r

overrides the initial translational temperature for each species
default is thermal equilibrium from the inlet file
input is one temperature (K) per species per line

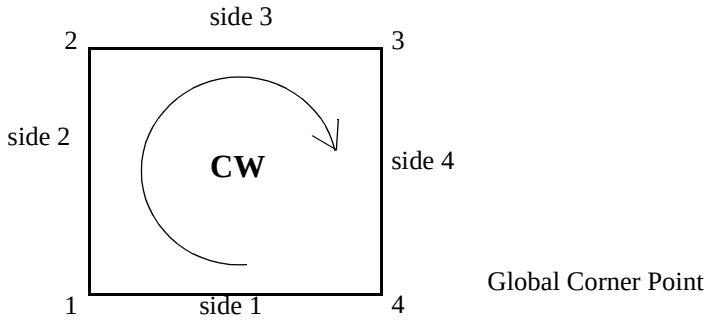
volume multiplier r

multiplies the actual region volume
This option is used to with an option for a surface to allow a better simulation of a 3D system with a 2D, axisymmetric code.

and a required input block:

grid

a> Four global corner points define the region. A region is a general quadrilateral and not required to be rectangular. Sides 1 and or 3 can be linear or quadratic (as in the sphere example); sides 2 and 4 MUST be linear. A diagram describing the layout of a region with regards to side and global corner point definition is shown below. Definition of the region sides and corner points is by a clockwise rule. In general the first corner point defining the region will be the lower left hand point (1) followed by points 2,3, and 4 respectively (clockwise direction). Sides 1 will always be defined as the side between global corner points 1 and 4 respectively. The other sides are defined in a similar fashion. Side 1 and 3 should be nominally parallel to the x or z axis. Sides 1 and 3 must not be vertical lines in the z-r or x-y plane. The example section of the manual illustrates several different ways



to 'build' a geometry by these region blocks. Note that a region side can share one or more region sides or a mix of regions and surfaces.

There are several options which can be invoked for the corner points.

"sticky points" (options 1 or 2)

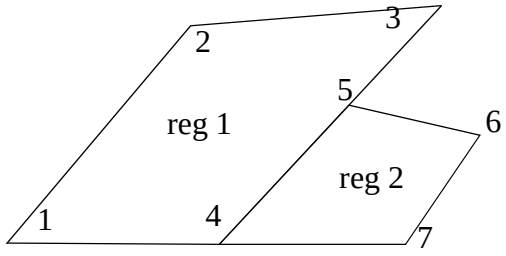
Sticky corner points are typically used when a region's corner point lies along the line of the adjacent region (see figure). To prevent a domain void from occurring, one would have to make sure that the corner point was exactly along the adjacent line; this point would have to be recomputed is the geometry was changed. The sticky point method allows for a point to be 'stuck' to an adjacent line; that is, for a given x value, the y value will be computed such that it is along the line or vice versa. A requirement is that the region to be 'stuck' have a lower region number since the code initializes the geometry a region at a time. The "stuck" region side can be either linear or quadratic. The syntax is:

(-corner pt. #) (region to 'stick' to) (side of this region) (1 or 2)

where: the corner point is entered as the negative of its actual value

1 == constant x value and the code will compute the y intersection

2 == constant y value and the code will compute the x intersection.



reg 1 corner pts.
1
2
3
4

reg 2 corner pts.
4
-5 1 4 1
6
7

corner pt. 5 for this example == (x value from input pt #5, y value calculated to intersect side 4)

"point-slope"(option 3)

This is option is a variation of the "sticky point" option. Now the corner point is determined from the intersection of a line determined by an input point and an input slope and a designated side of a region. Again, the designated region must have been defined before this region. The syntax is:

(-corner pt. #) (designated region) (region side) (3) (slope of intersection line)

b> Number of cells along sides 1 and 3. The same number of cells will be specified for the side pairs of (1,3) and (2,4). If you select 50 cells for side 1 of region 1 then there will also be 50 cells for side 3 of region 1.

c> Number of cells along sides 2 and 4.

d> The type of line/curve for sides 1 and/or 3

- 0 - a straight line for both side 1 and 3
  syntax: 0
- 1 - side 1 and 3 are quadratic with the center along the centerline (z axis)
  syntax: 1
- -1 - side 1 and 3 are quadratic with the center at the input pt. from the corner pt. list.
  syntax: -1 15 where: 15 is the corresponding pt. in the corner pt. list
- -3 - side 1 is quadratic and side 3 is linear with the center at the input pt.
  syntax: -3 15
- -4 - side 1 is linear and side 3 is quadratic with the center at the input pt.
  syntax: -4 15
- -5 - side 1 is quadratic with an input radius and side 3 is linear . Also the type of curvature (convex or concave) (0 or 1), the strategy for blending the intra-region grid lines from quadratic to linear (1, 2, or 3) are also required. If option 3 is used, then a power series factor controlling how fast the radius increases from the quadratic side to the linear (radius == infinity) is also an input.

syntax: -5 0 1
-5 1 2
-5 1 3 1.1

-6 - side 3 is quadratic and 1 is linear with the same input format as option -5.

e> Cell Spacing along sides 1 and 3. Spacing of the cells either can be uniform or the cells can be clustered to one or both ends.

0 - Uniform spacing

1 - Manually assign cell spacing via cell weights, 30 per line following this input line

2 - Cluster cells toward the lower number of side; that is, towards side 2.For this option, two additional inputs are required. The first specifies the size variation from cell to cell using a simple geometry ratio. For a value of 1.03, a 3% cell size variation will be obtained. The second sets the ratio of maximum to minimum cell size. This limits the smallest cell size.
syntax: 2 1.05 100.

3 - Cluster cells toward the higher number side or side 4. The inputs are the same as for option 2.
syntax: 3 1.03 200.

4 - Cluster cells towards both sides (2 and 4). The inputs are the same as for option 2.
syntax: 4 1.05 150.

f> Cell Spacing along sides 2 and 4. Spacing of the cells either can be uniform or the cells can be clustered to one or both ends. The syntax is the same as for the proceeding option.

g> Boundary conditions for sides 1 through 4 are specified. Each side must have a specific boundary condition type.

1	Line of symmetry (rz axis)
2	Line of symmetry (xy axis)
3	Constant freestream bc from the inlet table
+/-3x	Freestream bc using an inlet table.
5	Solid surface
+/-5x	Solid surface with sources from an inlet table
7	Connection to another region or multiple regions
+/-7x	Region connection with sources from an inlet table
9	Porous wall (porosity specified in the variable, value, on surface info. #45) or mixed boundary type (solid surface and region connectivity)
+/-9x	Porous wall or mixed boundary with sources from an inlet table
11	Outflow (non-reentrant, vacuum pump of infinite speed) (note type 11 cannot be used for a region connection)
12	Same as type 9. Computes net flux on type 9 if a type 12 bc is adjacent. (note: typically have type 9 BC as the ‘upstream’ boundary and 12 as the ‘downstream’ boundary) - MUST have a 9-12 pair
13	zero-gradient outflow (Neumann-like). The code computed the Maxwellian dist. from the upstream cell and samples from this distribution to obtain the particles to inject back into the domain to yield a zero-gradient boundary

Boundary types +/-3x, +/-5x, +/-7x,and +/-9x require a table entry be specified for 'x'. This specifies the table number to refer to in the *inlet* file. The boundary condition type can be + or -; positive number indicates that coordinate specified in the *inlet* file is either x or z, a negative boundary condition indicates that the coordinate is either y or r. Examples are: -51, and 32.

h> Number of surface specification input lines (#46). Required for boundary conditions 5, 5x, 9 and 9x.

i> Surface specification input variables on each line are:

1 - Region side number

2 &3 - Define the starting and stopping cell number for this specification.
note: this feature can input piecewise property variations along a surface
--cells are numbered as:
side 1-- cell 1 adjoins side 1-2 intersection
side 2 -- cell 1 adjoins side 1-2 intersection
side 3 -- cell 1 adjoins side 2-3 intersection
side 4 -- cell 1 adjoins side 1-4 intersection

4 - The number of evenly spaced surface elements per cell. This option can be used to greatly increase the accuracy of the solution of the Poisson Electro-statics equation by the Boundary Element Method without the tremendous cpu time penalty incurred by simply increasing the number of cells.

5 - Amount of specular reflection in Maxwell Model (0.0 for fully diffuse) (Chapter 1)

6 - Temperature of the surface (K).

7 - Material number associated with material number defined in the *surf_bc* file. (input 0 if no surface chemistry). A number without a *surf_bc* input can be used to 'mark' a particular surface for postprocessing with **surface2d**.

8 - Porosity for boundary type 9 and 9x (value of 1.0 for freeflow, 0.0 for no flow) (input 0.0 for boundary conditions other than type 9)

Note: to define a linear variation of temperature and/or porosity:

1-use a line entry for each 'end point' of the linear range (cell number domain)

2-set the region side number (first entry) to negative....

3-both temperature and porosity will be varied linearly between the endpoints

j> Region connectivity table. In most cases, multiple regions will need to be connected to define the specific geometry.

There are four rows in the region connectivity table, one for each side. The entries are:

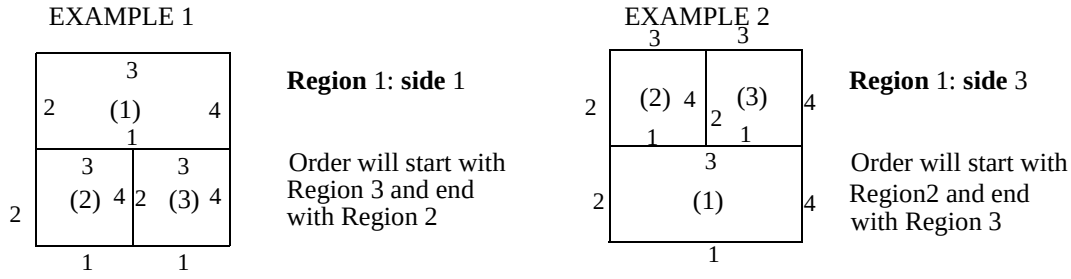
1 - side number

2 - the number of connecting regions to this side. For example, if a side is a solid surface there are no connecting regions and the entry is 0.

If 2nd value is non-zero, then there must be ((input 2)*2) numbers to follow, one pair for each connecting region.

3 - input pair which specify the connected region side number and region number in clockwise fashion for that side (see example below).

The diagram below shows two examples of region connectivity based on the clockwise rule.



In example 1, regions 2 and 3 are connected to side 1 of region 1. Applying **the clockwise rule** results in a region numbering sequence 3 and 2 on side 1 of region 1. Similarly, in example 2, regions 2 and 3 are connected to side 3 of region 1. In this case the connectivity order will be regions 2 and 3 to side 3 of region 1.

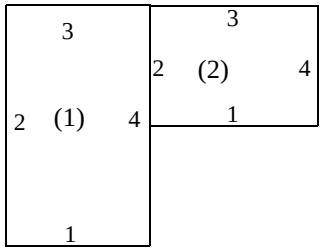
Example 1 - region 1 connectivity input for side 1:

12 3 3 3 2

Example 2 - region 1 connectivity input for side 3:

32 1 2 1 3

Boundary type 9 allows for multiple boundary type specification; for example side 4 of region 1 is connected to another region and is partly a solid surface:



boundary type for side 4 of region 1 == 9

surface specification (input #45) is required for side 4-- the porosity variable is used for the connecting side (1.0 for freeflow between the regions)

example: 4 1 50 0.0 300. 0 0.95

(the surface is defined to be at 300K and a porosity of 95% is used ONLY for the portion which connects to region 2. You do not have to have the region cell boundaries lineup on the region1-region 2 interface. The code logic will determine the correct particle trajectory. Also, the cell range of 1-50 simply needs to be inclusive of the actual number of cells.)

Example region connectivity for side 4 of region 1:
4 2 2 2 2 -1

Note: a pseudo-region, -1, is used to indicate where the solid surface is. Alternating regions and pseudo-regions can be used to build complex geometries (see samples section).

3.5 Species File Description (spec)

Example file:

```
****************************************
*      species data file           *
****************************************
6          number of species
*
3          internal structure of most complex molecule:
*          3-monatomic, 4-rotation, 5-rotat. + vibrat.
*
1          # of chemical reactions
*
*
*   NOTE:  Fe- electron mass increased by 1000 ---- use ONLY for steady state simulations!!!!
*
*-------------------------------------------------------------------------------------------------------------
*  ID
*  Mwt    Mol. mass   Diam.   #Rot.Deg.    Rot.Rel.  # Vib. Deg.  Vib. Rel. Vib.Temp. specie wt. charge   omega   tref   alpha
*           (kg)       (m)     Freedom      Coll. #    Freedom      Coll. #     (K)
*-------------------------------------------------------------------------------------------------------------------------
*
D2
  4.02     0.668e-26  0.2701e-9        0.0        0.0          0.0        0.0         0.0         1.0         0.0      0.67      300.   1.0
D
  2.01     0.334e-26  0.2211e-09       0.0        0.0          0.0        0.0         0.0         1.0         0.0      0.67      300.   1.0
D2+
  4.02     0.668e-26  0.2701e-9        0.0        0.0          0.0        0.0         0.0         1.0         +1.0     0.67      300.   1.0
D+
  2.01     0.334e-26  0.2211e-09       0.0        0.0          0.0        0.0         0.0         1.0         +1.0     0.67      300.   1.0
Fe-
  5.45e-4  0.9049e-27 6.941e-8        0.0        5.           0.         0.0         0.0         1.0         -1.0     1.0       300.   1.0
e-
  5.45e-4  0.9049e-30 6.941e-8        0.0        5.           0.         0.0         0.0         1.0         -1.0     1.0       300.   1.0
*
END
*
```

- Lines beginning with '*' are comments and are not used.
- The **first** data entry MUST be the number of species to input.
- The **second** data entry MUST be the number of degrees of freedom which describes the most complex molecule.
  - 3 - translational modes (one for each direction)
  - 4 - rotational + translational modes (for diatomic molecules)
  - 5 - vibrational + rotational + translational modes

    The default model is for a single vibrational *temperature*; quantized models are also available

- The third data entry MUST be the number of chemical reactions to be read in. The chemistry filename will be chem (default) or user provided by the 'chemistry file' input option.

- The next data section describes each species. **The order of the species in this file is very important; this order is assumed throughout the calculation.**

  Each species requires two lines of input.

  line 1: species chemical symbol (used in postprocessing files, 6 characters long)

  line 2: description of the species for transport and interactions:
  molecular weight, molecular mass (kg), molecular diameter (m),
  # of rotational degrees of freedom, rotational relaxation collision number,
  # of vibrational degrees of freedom, vibrational relaxation collision #,
  vibrational temperature, species weight (described below), charge number,
  omega (collision model - viscosity), reference T (K) for omega and alpha,
  alpha (VSS collision model - diffusivity) .

  If either not modelling or have no information for rotational/vibrational interactions, enter 0.0.

  Species weighting is a strategy used to increase statistics on species that exist in low concentrations. Only two different specie weights are allowed: 1.0 and a number < 1.0. In the example, you will see that either 1.0 or 0.02 are used for species weight. A species weight less than 1 multiplies the cell ratio of the # of real molecules per simulated one. For example, consider a mixture of 2 species: one with a mole fraction of 0.99 and the other 0.01. If the weights were equal to 1.0 for both species and there were 100 computational particles in the cell, 99 would be species 1 and 1 particles would be species 2. Thus, if there were only 20 particles in the cell, on the average, the 20 particles would all be species type 1! If the species weight was 0.02 for species 2, then on the average, the cell would have 14 particles of species 1 and 6 of species 2. **Species weight must be a number between 0.0 and 1.0!**

  By default, interspecies omega and alpha are simply the arithmetic average of the individual species values. If information is available, these defaults can be overridden in the following optional input section.

- This is the optional input section:

  alpha i j r
  This is used to override the default arithmetic average for an alpha for species i and j with value r.

  omega i j r
  This is used to override the default arithmetic average for an omega for species i and j with value r.

  tref i j r
  This is used to override the default arithmetic average for a tref for species i and j with value r.

vibration model i

Flag to use a different vibrational model (temperature dependent relaxation) such as the Miliken & White model. The model will be user supplied; an example can be found in the *eos.f* code module. (default value = 0)

rotational model i

Flag to use a different rotational model (temperature dependent) such as the Miliken & White model. The model will be user supplied; an example can be found in the *eos.f* code module. (default value = 0)

- The last input line MUST be **END**.

3.6 Inlet File Description (inlet)

Example *inlet* files. An asterisk, *, in column 1 denotes a comment line. **An *inlet* file is required if you specified an inlet as a boundary condition in the *geometry.inp* file or are specifying initial conditions for the computational domain.** (an *inlet* file is required for BC types: 3, +/-3x, +/-5x, +/7x, +/-9x).

example 1

```
*
*-- 15sccm -- point source -- new grid2
*
2           number of tables
*
1    1      1     1      table number, # multiple tables, number of entries, BC type
*           #/ s
-0.038   6.7179e+18   0.00   -199.725 255.79   255.79  255.79  0.  0. 0. 1.0  0. 0.
*
*-- 15sccm distributed over the outer-ring radius, outgassing boundary condition
2    1      2     2      table  number, number of entries
*  location  #/m2s    Vz     Vr         Tt       Tr         Tv         species fractions
-0.001      2.669e20    0.0     0.0       300.     300.      300.   0.0  0.0  0.0  1.0  0.0  0.0
-0.033      2.669e20    0.0     0.0       300.     300.      300.   0.0  0.0  0.0  1.0  0.0  0.0
```

example 2

```
*
*   freestream/initial inlet condition for the ICF sphere
*
*      Xe species
*
1 number of tables
*
0   -----  flag to specify freestream/initial conditions
3.216e20   400.    0.0     1500.   1500.   1500.    1.
*
```

example 3

```
*
*    inlet for Ion Accelerator--- geom 1
*      D2  D   D2+   D+   Fe-    e-
*
3 number of tables
*
0           initial conditions
*           #/m3       Vx      Vy      Tt     Tr       Tv      Ni.....
          1.e18        10.    0.0      23200.  0.0    0.0     0.0    0.1   0.0   1.0   1.0  0.0
*
1    1      2     2    --   table#, multiple table entry #, # entries, BC type
*      entry for neutrals at edge of sheath
*           #/m^2-s
```

```
 0.000    1.0e24    9.3e5  0.00    23206.  23206. 23206. 0.0  0.1  0.0  1.0 0.0  0.0
 0.00056  1.0e24    9.3e5  0.00    23206.  23206. 23206. 0.0  0.1  0.0  1.0 0.0  0.0
*
1   2    2    2
*
 0.000    1.0e24    2.9e4   0.00    1.  1. 1. 0.0  0.0  0.0  0.0 1.0  0.0
 0.00056  1.0e24    2.9e4   0.00    1.  1. 1. 0.0  0.0  0.0  0.0 1.0  0.0

*
```

File Description

line 1: Number of tables to be read (number of separate inlets).

for each table:

first line: Table number, # in multiple table, number of entries, table type

table number: sequential number only used for ordering the input

if == 0, this is a flag to indicate initial domain and freestream conditions for a boundary condition type 3 (*volume source*). There are no other inputs on the first line for a table number 0 (see above example 2).

multiple tables: Multiple inlet boundary conditions can be defined for a given surface--for example, a two stream, two specie source where the fluxes and temperatures were different for each species. Simply enter a table entry for stream source and index the 2nd number in the first line (multiple table option): the multiple table option would be '1' for the first stream source, '2' for the second, etc (see above example 3). Note that both multiple tables are numbered '1'. The '# in multiple table' must be sequential and incremental: 1,2,3.etc.

number of entries: the number of entries for that inlet table. The entries between the input locations are linearly interpolated; to input a inlet profile, simply use more entries for the table.

table (boundary condition) types:

1 -- point source, #/s (1 sccm = 4.48e17 #/s)

2 -- surface flux, #/m^2-s

(note--a unit depth of 1m is assumed in cartesian (XY) coordinates)

3 -- volume source, #/m^3

next lines:single input line for each table entry

- inlet location, BC type specifies coordinate (m)

The inlet location can be either x or y (z or r in axisymmetric systems). A single coordinate is used since the inlet boundary conditions must be along a region boundary; the **init2d** code determines the second coordinate to machine

accuracy. If the BC type code specified in *geometry.inp* is negative (i.e. -31, -52, -93, etc.) then the inlet location coordinate is assumed to be either y or r. If the BC type code is positive, the inlet coordinate is either x or z.

- flow rate (units depend on the BC type)
  - boundary types: 3x, 5x, 7x, or 9x, each can have either a 1, or 2, or 3 type boundary.
  - for a point source (+/-5x), 1sccm = 4.48e17 #/s
  - multiple point sources can exist along a boundary
  - For BC 2 and 3, linear interpolation is used between input values; profiles are modelled as a series of line segments.
  - BC type +/-3x is generally used for a 'line' inflow boundary condition
  - BC type +/-5x if for a point source (small inlet nozzle - code 1) or for an outgassing surface (code 2).
  - BC type +/-9x is for the special case where a region has both a surface and region connection on the *same side* or for a porous connection between regions.

- Vx or Vz average inlet velocity vector (m/s)

  The input velocities are the average velocities; the translational temperature is used to obtain the velocity distribution which is sampled for the inlet particle velocity.
  - use standard sonic flow relationships (see Chapter 10) to obtain both orifice velocities and exit temperatures (V* and T*)
  - make sure that the velocity vectors are **into** the computational domain!

- Vy or Vr average inlet velocity vector (m/s)

- Translational Temperature (K for non-electrons, eV for electrons)

  NOTE: for table number = 0 (initial/freestream conditions), the translational temp. is in K for all species (init2d will convert to eV if electron species are present)

- Rotational Temperature (K)

- Vibrational Temperature (K)

- species mole fractions in same order as *geometry.inp* and *spec* file

3.7 Surface Boundary Condition File (surfbc)

The surface boundary condition file contains a separate table for each type of material specified in the *geometry.inp* file. An asterisk, *, in column 1 denotes a comment line. This file controls both surface chemistry, translating/rotating walls, applied potentials, and other boundary inputs. They are differentiated by the line 1 input: the boundary condition type variable.

Surface reaction probability can be defined with a simple sticking coefficient or it can be a function of site coverage. The surface coverage model is simple: sites are either occupied or vacant. Thus, only one type of surface species can be defined. Ion energy sputtering yield can also be described for a surface reaction using the expression $A(E^a_{ion} - E^a_{th})^b$ as defined by Gray et al. (*J. Vac. Sci. Technol. A*, vol. 12, pp. 354-364, 1994). In the event that a product is not formed during an ion surface reaction an alternate reaction product can be specified to insure ion neutralization.

For Example:

$CF3^+ + SiO_2\text{-Coverage}_{(surface\ site)}$ -------> $SiF_4 + CO_2$ **or** CF_3

Example surfbc input files:

example 1

```
*
*  this file contain surface chemistry information for the Poisson test  - H2 chemistry
*      D2  D2+    D    D+   e-
*      1    2       3     4    5
*
*  variable order for each reaction:
*  (Rx type) (Species-i) (Species-r1) (Species-r2) (create prob-1)
*   (create prob 2) (degree of specular reflect) (Rx prob)
*
* For type 8:  type icode voltbc eps1 eps2 0. 0. 0.
*
3   number of material table types
*
* material 2  voltage=100V
2  1   1.4e16
8.  1.  100.  0.   0.0   0.  0.    0.0
*
* material 3, mirror bc (Enormal = 0), specular
3  1   1.4e16
8.  2.   0.  0.   0.0   0.  0.    0.0
*
* material 4  voltage=10V
4  1   1.4e16
8.  1.  10.  0.   0.0   0.  0.    0.0
```

example 2

```
*
*  this file contain surface chemistry information for tube2 - H2 chemistry
*       D2  D2+    D    D+   e-
*       1    2        3     4     5
*
*  variable order for each reaction:
*  (Rx type) (Species-i) (Species-r1) (Species-r2) (create prob-1)
*   (create prob 2) (degree of specular reflect) (Rx prob)
*
* For type 8:  type icode voltbc eps1 eps2 0. 0. 0.
*
10  number of material table types
*
* material 1 screen plate -- voltage=0KV, ions neutralize, e stick
1 5  1.4e16
1.  2.   1.  0.   1.0   0.  0.    1.0            D2+  -->  D2
1.   3.    1.  0.   0.5    0.0   0.0     0.1      D    -->  D2
1.  4.   3.  5.   1.0   1.5  0.    1.0           D+   -->  D + 1.5e-
1.  5.   5.  0.   0.0   0.  0.    1.0           e-   -->  stick
8.  1.   0.  0.0  0.0   0.  0.    0.0
*
* material 2 accel. plate -- voltage=-100kV, ions neutralize, e stick
2 5  1.4e16
1.  2.   1.  0.   1.0   0.  0.    1.0
1.   3.    1.  0.   0.5    0.0   0.0     0.1      H --->  H2
1.  4.   3.  5.   1.0   1.5  0.    1.0
1.  5.   5.  0.   0.0   0.  0.    1.0
8.  1.  -100000.0  0.0  0.0   0.  0.    0.0
*
* material 3, source -- 5 voltage bc, all sticks- electrons reflect
3  5   1.4e16
1.  2.   1.  0.   1.0   0.  0.    1.0            D2+  -->  D2
1.   3.    1.  0.   0.5    0.0   0.0     0.1      D    -->  D2
1.  4.   3.  5.   1.0   1.5  0.    1.0           D+   -->  D + 1.5e-
1.  5.   5.  0.   1.0   0.  1.    1.0           e-   -->  reflect
8.  1.   5.  0.0  0.0   0.  0.    0.0
*
* material 4, dielectric (Neumann for now)
4  4   1.4e16
1.   3.    1.  0.   0.5    0.0   0.0     0.1      H --->  H2
1.  4.   3.  5.   1.0   1.5  0.    1.0
1.  5.   5.  0.   0.0   0.  0.    1.0
****8.  3.   0.  1.   9.0   0.  0.    0.0
8.  2.   0.      0.    .0   0.  0.    0.0
*
* material 5, target -- time dependent voltage bc
*  secondary electron emission
5  6   1.4e16
1.  1.   1.  0.   0.0   0.  0.    1.0
1.  2.   2.  0.   0.0   0.  0.    1.0
1.  3.   3.  0.   0.0   0.  0.    1.0
```

```
1.  4.   3.  5.   1.0   1.5  0.    1.0
1.  5.   5.  0.   0.0   0.  0.    1.0
8.  5.  00.0  0.5   300.0   -100000.  0.    0.0
*
* material 6, mirror bc (Enormal = 0), specular
6  1   1.4e16
8.  2.   0.  0.   0.0   0.  0.    0.0
*
* material 7 accel. plate  back side- ions neutralize, e stick
7 4  1.4e16
1.  2.   1.  0.   1.0   0.  0.    1.0
1.   3.    1.  0.   0.5    0.0   0.0     0.1       H --->  H2
1.  4.   3.  5.   1.0   1.5  0.    1.0
1.  5.   5.  0.   0.0   0.  0.    1.0
*
* material 8 backside of target -- voltage=0, ions neutralize, e stick
8 5  1.4e16
1.  2.   1.  0.   1.0   0.  0.    1.0
1.   3.    1.  0.   0.5    0.0   0.0     0.1       H --->  H2
1.  4.   3.  5.   1.0   1.5  0.    1.0
1.  5.   5.  0.   0.0   0.  0.    1.0
8.  6.  00.0  0.5   120.0   0.  0.    0.0
* material 9 --- internal structures 0V- slow ions -- expansion region
9.  5.  1.75e19
1.   4.    3.  0.   1.     0.    0.0     0.5       H+ -->  H
1.   3.    1.  0.   0.5    0.0   0.0     0.1       H --->  H2
1.   2.    1.  0.   1.     0.    0.      0.5       H2+  -->  H2
1.  5.   5.  0.   0.0   0.  0.    1.0
8.  2.  0.0  0.0  0.0   0.  0.    0.0
* material 10 --- external walls 0V- slow ions  -- expansion
10.  5.  1.75e19
1.   4.    3.  0.   1.     0.    0.0     0.5       H+ -->  H
1.   3.    1.  0.   0.5    0.0   0.0     0.1       H --->  H2
1.   2.    1.  0.   1.     0.    0.      0.5       H2+  -->  H2
1.  5.   5.  0.   0.0   0.  0.    1.0
8.  1.  0.0  0.0  0.0   0.  0.    0.0
```

File Description

Line 1: Number of material tables

For each table:

first line: Table number, number of entry sets per table, site density(#/m^2).

Table number: identifier used in the input file for the surface definition. The order is not important

number of entries: the number of data sets (not necessary lines) per table. A data set can be either one or two lines.

site density: only used for surface dependent chemistry (coverage model). if not, use any input value

data sets (either one or two lines per material)

•required input line(A) required for all BC types **(8 real entries)**

boundary condition types +/-1 thru +/-8): Types 1 thru 6 specify surface chemistry where a positive reaction type indicates that the reaction rate is not temperature dependent and no ion energy dependent yield information is required. A negative reaction type indicates an extra line is read in to allow for surface temperature dependence and for ion energy dependent yield parameters. Type 7 is a translating/rotating boundary. Type 8 indicates boundary conditions to be used in the Poisson electrostatic field solver. Note that all boundaries defining the fields must be specified as surface elements once and only once; that is, if a zero width structure is in the domain, do not have surface elements with electrostatic boundary conditions on both sides.

entry1: BC **type**:

+/-1	Simple model (no coverage dependence)
+/-2	Absorption reaction - takes open surface site.
+/-3	Etch reaction - vacates occupied surface site.
+/-4	Requires an open site but leaves the surface unchanged.
+/-5	not used at this time
+/-6	not used at this time
+/-7	translating or rotating boundary
8	boundary condition used for electrostatics (Poisson field solver)

For BC **types 1 through 6** (surface chemistry):

entry 2: reacting species number (corresponding to *spec* and *geometry.inp* files)
entry 3: reaction product species #1
entry 4: reaction product species #2 (specify 0. if only one reaction product)
entry 5: creation probability species #1
entry 6: creation probability species #2
entry 7: degree of surface specular reflection (0.0 for diffuse)
entry 8: Surface reaction probability (A)

For BC **type +/-7** (translating or rotating surface):

entry 1: +7 translating surface (cartesian coordinate system)
-7 rotating surface (axisymmetric coordinate system)
entry 2: u-velocity (x-direction), m/s (for translating surface)
entry 3: v-velocity (y-direction), m/s (for translating surface)
entry 4: rotational speed , rev/s (MUST be axisymmetric coordinate system)
entry 5: 0.0
entry 6: 0.0
entry 7: 0.0

entry 8: 0.0

For BC **type 8** (electrostatic BC):

entry 2: *icode* to specify the type of BC for the Poisson electrostatic solver:

- 0 = surface NOT included in electrostatics calcs.
- 1 = applied potential, volts (direchlet)
- 2 = surface normal field is zero (neumann)
- 3 = dielectric material (not currently implemented)
- 4 = time varying surface potential (AC) superimposed on DC potential
  $V(t) = V_{DC} + V_o \sin(2 \pi \omega t)$
- 5 = a current based bc.....requires resistance drop to a constant voltage
- 6 = 'backside' boundary for icode=5 .... allows a bc without a surface charge element
- 7 = periodic bc -- electrically equivalent to icode =2
- 8 = surface element with constant potential -- value from runtime input
- 9 = flag for an icode=1 element internal to domain....code reverses the surface unit normal and changes it to an icode=1 element
- <0 = floating conductor (computes surface charge and redistribution on a constant voltage surface) (not verified)

entry 3: if (icode.eq.1) applied potential, volt,
else set to 0.0

entry 4: if (icode.eq.4) then its the magnitude of the AC component (volts)
if (icode.eq.5) then its the backward time averaging factor
=1 for implicit (no time averaging)
else set to 0.0

entry 5: if (icode.eq.4) then its the rf frequency (Hz)
if (icode.eq.5) then its the resistance to a constant potential
else set to 0.0

entry 6: if (icode.eq.5) then its the constant potential via the resistance, volt
else set to 0.0

entry 7: 0.0

entry 8: 0.0

For BC **types -1 through -6** (surface chemistry):

entry 2: reacting species number (corresponding to *spec* and *geometry.inp* files)

entry 3: reaction product species #1

entry 4: reaction product species #2 (specify 0. if only one reaction product)

entry 5: creation probability species #1

entry 6: creation probability species #2

entry 7: degree of surface specular reflection (0.0 for diffuse)
entry 8: Surface reaction probability (A)
Additional line(B) for surface reactions with temperature dependence or ion energy dependence (7 entries on second line)

entry 1: B - surf. reaction temperature dependence
(for Arrhenius fit $K = AT^B e^{(Ea/T)}$)
entry 2: Ea (joules) - surf. reaction activation energy
entry 3: A - energy dep. etch yield in the form of $A(E^a_{ion} - E^a_{th})^b$
entry 4: a - energy dep. etch yield parameter
entry 5: b - energy dep. etch yield parameter
entry 6: Eth (joules) - energy dep. etch yield threshold energy
entry 7: alternate reaction product, species #1

The creation probability contains reaction stoichiometry information; for Cl etch to create $SiCl_2$ the creation probability is 0.5 because it will only form once for two Cl's that hit the surface. (Cl --> 1/2 $SiCl_2$..... the 1/2 is the creation probability per incident particle)

examples:

•Cl recombination to Cl_2 can be described as either an overall reaction with a wall recombination coefficient of 0.1 for Cl --> 1/2 Cl_2 (fully diffuse reflected product):

```
1.  1.   4.    0.   0.5   0.   0.    0.1
```

Or, Cl recombination can be described as a two step process dependent on surface coverage:

Cl + Si(s) -> SiCl(s) (reaction type 1)

Cl + SiCl(s) -> SiCl2(g) + Si(s) (reaction type 2)

```
2.  1.   0.    0.   0.0   0.   0.  1.0
3.  1.   4.    0.   1.0   0.   0.  0.05
```

An example of temperature dependent etching rate is given for C2F6 etch of SiO2

```
*    OMEGA C2F6 plasma simulations with 10 rnxs, 11 species
*  C2F6  F2   CF3   F   F+   CF3-  SiF4   CF2  CF2+  CF  CF+   O2  CO2  CF3+
*   1      2      3   4   5      6      7      8      9      10  11     12  13    14
1     number of material table types
*
* material 1 (oxide wafer SiO2 etch)
1  9  1.75e19
2.   4.   0.     0.    0.0  0.0 0.0  0.2
2.  10.   0.     0.    0.0  0.0 0.0  0.33
```

```
2.  8.  0.    0.   0.0  0.0 0.0  0.33
2.  3.  0.    0.   0.0  0.0 0.0  0.33
-3. 14.  7.    13.  1.0  1.0 0.0  1.0
 0. 0.  .053  .5  1.0  6.4e-19   3.
-3. 5.  7.    12.  1.0  1.0 0.0  1.0
0. 0.  .053  .5  1.0  6.4e-19   4.0
-3. 9.  7.    13. 1.0  1.0 0.0   1.0
 0. 0.  .053  .5  1.0  6.4e-19   8.
-3. 11.  7.   13. 1.0  1.0 0.0 1.0
0. 0.  .053  .5  1.0  6.4e-19    10.
1. 6.   6.   0.    1.0  0.0 1.0  1.0
```

Example *surf_bc* file:

```
*
*  this file contain surface chemistry information for the
*  UH - GEOM1 Problem  Cl2 chemistry
*      Cl,    Cl+  , Cl-,  Cl2,  Cl2+,  SiCl2
*      1         2        3         4    5     6
*
2      number of material table types    etch of Si -->  SiCl2
*
* material 1 (wafer), wafer
1. 7.  1.75e19      table number, number of entries(reactions), site density(#/m2)
* Following input defines surface reactions on material type #1
*First two reactions are Cl recombination to Cl2 with surface coverage
*           dependence (see explanation below)
2.  1.   0.    0.   0.0    0.   0.  1.0
3.  1.   4.    0.   1.0    0.   0.  0.05
* Next reaction is Cl- reflecting at wall fully specular due to sheath.
1.  3.   3.    0.    1.0   0.0   1. 1.0
* Cl+ and Cl2+ ion etching (doesn't include values for energy dependent
*                                etch yield)
3.  2.   6.0   0.    1.0   0.    0. 1.0
1.  5.   6.0   0.    1.0   0.    0. 1.0
*
* material 2, upper head
2.  4.  1.75e19
1.  1.   4.    0.   0.5    0.    0. 1.0
1.  2.   1.    0.    1.0   0.0   0.  1.0
1.  3.   3.    0.    1.    0.0   1.  1.0
1.  5.   4.    0.    1.0   0.0   0.   1.0
```

3.8 Cross Section File (cross_section)

This file is used to specify a constant cross-section for a particle-particle interaction instead of the default VHS model. For cross-sections not specified in this file, the VHS model will be used. It can also be used to input a chemical reaction rate or interaction event in a JANEV 9-order polynomial fit format. An asterisk, *, in column 1 denotes a comment line.

Example *cross_section* files:

example 1

```
*    cross section input file - overwrite the VHS based values
*    file for charged particles and neutral
*
9       0
2  1
100.e-20
2  4
100.e-20
2  6
100.e-20
3  1
100.e-20
3  4
100.e-20
3  6
100.e-20
5  1
100.e-20
5  4
100.e-20
5  6
100.e-20
```

example 2

```
*    cross section input file - overwrite the VHS based values
*
*     first line == # constant inputs, # reaction fits
*    note:   ICARUS in SI....so sigma in m**2.....
*
0     1
*
*   charge exchange rx. for :   p + H(1s)  --->    H(1s)   +  p
* fit#  type    Emin      sigma(Emin)      sigmax      multiplier
  1        6          0.1        7.e-15               7.e-15       1.e-4       (in cm**2)
*   fits for #1
-3.27412379e1    -8.9164565e-2    -3.01699076e-02     9.2054824e-3   2.40026656e-3
-1.92712231e-3   3.65475034e-4    -2.78886646e-5      7.422296363e-7
```

File Description

line 1: (# of constant cross-section entries) (# of fits)

for each constant cross-section entry (these MUST be before any fit entries)

first line: species pair numbers as defined by the order in the spec file.
second line: constant collision cross-section (m^2)

for each fit entry

first line: 6 entries

entry 1: fit number (referenced from the chemistry file) (integer)
entry 2: fit type (integer) - must be type 6 at present

Fit 6: $\ln K = \sum_{i=1}^{9} k_i \cdot \langle \ln Te \rangle^{i-1}$

entry 3: for fit type 6 (JANEV), min energy to use fit (eV)
entry 4: for fit type 6, cross-section at min energy
entry 5: for fit type 6, maximum cross-section
entry 6: for fit type 6, multiplier to convert cross-section fit result to SI (m**2)

second line: k1, k2, k3, k4, k5
third line: k6, k7, k8, k9

3.9 Gas Phase Chemistry File *(chem or chem.asc)*

The number of gas phase reactions is defined in the *geometry.inp* file and must match the chemistry input file. Two formats are allowed for the chemistry input: the standard Icarus chemistry format as defined for the file (*chem*) or the standard Chemkin format (chem.asc). The default is the DSMC chemistry format; set the number of chemical reactions in the geometry.inp file to its negative for the Chemkin input option. A Icarus formatted file is also generated with the Chemkin option (output file == chem). The Chemkin file, chem.asc, is generated from user input by the Chemkin Interpreter (not included in this software package). An asterisk, *, in column 1 denotes a comment line.

Example file:

```
*Hydrogen Chemistry Input File: 2/4/1999
*       2/4/99: Electron Species included
*               Excitation energies corrected
*        Note multiplier on rate is 10-6, units for rate m^3.
*               Source of cross sections from "Elementary Processes in Hydrogen-Helium Plasmas", by,
*                                       R.K. Janev, et al, Springer Series on Atoms and Plasmas,
*                                               Springer-Verlag (Berlin, Heidelberg, New York) 1987.
*                                       web address for data:  www.iaea.org/programmes/amdis/ala/aladdin_7.txt
*
* updated for different product grouping - new init2d chemistry reader
*-------------------------------------------------------------------------
*  This input file contains the data characterizing the chemical reactions.
*  If input # reactions = 0, there is no chemistry, and this file is not read.
*     input lines are free format
*     the reaction equation is an input line (a25)
*-------------------------------------------------------------------------
*
*
* NOTE:  line 0 character string illustrating the reaction
*        line 1 defines rx. stoichiometry
*        line 2 for type 0, -1, & -2 MUST have 5 real numbers
*        line 2 for type -3 MUST have 2 integers and 1 real number
*        line 3 for type -3 MUST have 6 real numbers
*
*
*
*         first number on line 1 defines reaction type:
*
*              0 -- standard Arrhenius collisional chemistry k = A T^B exp(-Ea/kT)
*                   second line variables:
*                   1 -- number of internal degrees of freedom
*                   2 -- Ea
*                   3 -- A
*                   4 -- B
*                   5 -- heat of rx (+ for exothermic) - joules
*
*             -1 -- Charge Exchange reaction with fixed rate
*                   second line variables:
*                   1 -- 0 - constant, else == cross-secton input table #
*                   2 -- sigma CE (m^2)
*
*             -2 -- Charge Exchange reaction using model from Rapp & Frances(1962)
*                         sigma = ( k1 - k2*alog(vr) )**2
*                   second line variables:
*                   1 -- k1 for elastic collision
*                   2 -- k2 for elastic collision
*                   3 -- k1 for charge exchange
```

```
*                   4 -- k2 for change exchange
*
*              -3 -- Electron Impact reactions
*                   second line variables:
*                   1 -- equation type (if <0, T in K instead of eV)
*                   2 -- number of products (1 or 2)
*                   3 -- heat of formation (Frank-Candom)- joules
*                   third line variables:
*                   1 - 6 are fit coefficients
*
*
*
*   Hydrogen --- # 1   --------
*
*      D2   D2+  D    D+   e-
*      1    2    3    4    5
*
*  !!!!Mulitplier on Rates is 10-6 since rates in m^3 (cross sections m^2)!!!!!
*
*
*REACTION                          TYPENOTE
1. e + D2(GS)  => e + D(1s) + D(1s)Dissociation
-3     5    1    1   2     5    3   3
    6   0   0.96e-19  10.00
 32     1      1.26        3.25e-12      3.82e-9       1.e-6
  -2.858072836568e+01  1.038543976082e+01 -5.383825026583e+00 1.950636494405e+00 -5.393666392407e-01
  1.006916814453e-01 -1.160758573972e-02  7.411623859122e-04 -2.001369618807e-05
*
2. e + D2(GS)  => e + D(1s) + D(2s)Dissociation
-3     5  2  1  2  5  3   3
   6   0   0.96e-19 14.9
33     1      2.51        7.88e-12      6.92e-9       1.e-6
-3.454175591367e+01  1.412655911280e+01 -6.004466156761e+00 1.589476697488e+00 -2.775796909649e-01
3.152736888124e-02 -2.229578042005e-03  8.890114963166e-05 -1.523912962346e-06
*
3. e + D2(GS)  => e + D(2p) + D(2s)Dissociation
-3     5  1  1  2  5  3   3
  6   0   0.0  23.0
  34     1      5.01        6.48e-12      1.31e-9       1.e-6
   -4.794288960529e+01  2.629649351119e+01 -1.151117702256e+01 2.991954880790e+00 -4.949305181578e-01
 5.236320848415e-02 -3.433774290547e-03  1.272097387363e-04 -2.036079507592e-06
*
4. e + D(1s)     => e + (e + D+)Ionization
-3     5  3  1  2  5  4  5
  6  0   0.0  13.6
  25     1      2.0        7.22e-12       3.11e-8       1.e-6
  -3.271396786375e+01  1.353655609057e+01 -5.739328757388e+00 1.563154982022e+00 -2.877056004391e-01
  3.482559773737e-02 -2.631976175590e-03  1.119543953861e-04 -2.039149852002e-06
*
5. e + D(2s)     => e + (e + D+)Ionization
-3     5  3  1  2  5  4  5
  6  0  0.0  3.4
  26     1       0.398      8.87e-12        1.71e-7       1.e-6
  -1.973476726029e+01  3.992702671457e+00 -1.773436308973e+00 5.331949621358e-01 -1.181042453190e-01
  1.763136575032e-02 -1.616005335321e-03  8.093908992682e-05 -1.686664454913e-06
*
6. e + D2   => e + (e + D2+(v))Ionization
-3     5  1  1  2  5  2  5
  6  0 0.0  15.4
35     1      2.0         2.34e-12      5.18e-8       1.e-6
 -3.568640293666e+01  1.733468989961e+01 -7.767469363538e+00 2.211579405415e+00 -4.169840174384e-01
 5.088289820867e-02 -3.832737518325e-03  1.612863120371e-04 -2.893391904431e-06
```

```
*
7. e + D2   => e +  (e + D(1s) + D+ )Dissociative Ionization
-3   5  1  1  3  5  5  3  4
  6  0  0.0  18.0
36     1      3.98        3.74e-12      2.89e-9       1.e-6
 -3.834597006782e+01  1.426322356722e+01 -5.826468569506e+00 1.727940947913e+00 -3.598120866343e-01
 4.822199350494e-02 -3.909402993006e-03  1.738776657690e-04 -3.252844486351e-06
*
8. e + D2+(v)  => e + (e + D+ + D+ )Dissociative Ionization
-3   5  2  1  3  5  5  4  4
   6 0  0.0  14.7
 37     1      3.16        5.23e-12      9.06e-9       1.e-6
 -3.746192301092e+01  1.559355031108e+01 -6.693238367093e+00 1.981700292134e+00 -4.044820889297e-01
 5.352391623039e-02 -4.317451841436e-03  1.918499873454e-04 -3.591779705419e-06
*
9. e + D2+(v)  => e + D+ + D(1s)Dissociative Ionization
-3  5  2  1  2  5  4   3
   6  0  0.0  2.4
 38     1      0.2         1.23e-12      1.15e-7       1.e-6
 -1.781416067709e+01  2.277799785711e+00 -1.266868411626e+00 4.296170447419e-01 -9.609908013189e-02
 1.387958040699e-02 -1.231349039470e-03  6.042383126281e-05 -1.247521040900e-06
*
10. e + D2+(v)  => e + D+ + D(n=2) Dissociative Ionization
-3   5  2  1  2  5  4    3
  6   0  0.0  14.0
  39     1      2.0         5.03e-12      1.77e-7       1.e-6
   -3.178647420e+01  1.573560727511e+01 -6.992177456733e+00 1.852216261706e+00 -3.130312806531e-01
   3.383704123189e-02 -2.265770525273e-03  8.565603779673e-05 -1.398131377085e-06
*
11. e + D2+(v)  => D(1s) + D*(n)Dissociative Recombination
-3  5  2  0  2   3   3
 6  0  0.0  0.00
   40     1      0.1         2.23e-7       2.23e-7       1.e-6
 -1.670435653561e+01 -6.035644995682e-01 -1.942745783445e-08 -2.005952284492e-07  2.962996104431e-08
 2.134293274971e-08 -6.353973401838e-09  6.152557460831e-10 -2.025361858319e-11
*
12. D+ + D(1s)   =>    D(1s)   +  D+          Charge Exchange
-1        4     3      1    1    3   4
        1.0      7.e-15       0.   0.   0.
*
13. e + D(1s)   => e + D(2p)Excitation
-5  5  3  1  1  5  3
   6  0  0.0  10.2
   34     1      1.26        4.78e-12      3.18e-9       1.e-6
 -2.814949375869e+01  1.009828023274e+01 -4.771961915818e+00 1.467805963618e+00 -2.979799374553e-01
 3.861631407174e-02 -3.051685780771e-03  1.335472720988e-04 -2.476088392502e-06
*
14. e + D(1s)   => e + D(2s) Excitation
-5  5  3  1  1  5   3
   6  0  0.0  10.2
   34     1   1.26        3.54e-12      3.22e-9       1.e-6
-2.833259375256e+01  9.587356325603e+00 -4.833579851041e+00 1.415863373520e+00 -2.537887918825e-01
 2.800713977946e-02 -1.871408172571e-03  6.986668318407e-05 -1.123758504195e-06
*
15. e + D(2s)   => e + D(2p) Excitation
-5  5  3  1  1  5   3
   6  0  0.0  0.00001934
   34     1     0.1       1.18e-12      1.18e-9       1.e-6
 -1.219616012805e+01 -3.859057071006e-01 -6.509976401685e-03 4.981099209058e-04 -4.184102479407e-05
 3.054358926267e-06 -1.328567638366e-07  8.974535105058e-10  1.010269574757e-10
*
16. e + D2(v=0)  => e  +  D2(v=1) Vibrational Excitation
```

```
-5  5  1  1  1  5   1
   6  0  0.0  0.5
  34     1     0.158       5.83e-12      2.6e-9       1.e-6
 -2.017212494454e+01  9.563952280637e-01 -6.931474225637e-01 1.673671529631e-01 -3.228762898855e-02
 5.838603222226e-03 -8.580542691302e-04  7.456311623168e-05 -2.666978300757e-06
*
17. e + D2(v=0)  => e   +  D2(v=2) Vibrational Excitation
-5  5  1  1  1  5    1
   6  0  0.0  1.0
   34     1    0.398       5.93e-12      7.07e-10       1.e-6
-2.265507686305e+01  2.239943592222e+00 -1.099426577160e+00 2.339027647223e-01 -2.528511103871e-02
 6.851302489620e-04 1.253426182224e-04 -1.253475051672e-05  3.545892878015e-07
*
18. e + D2(GS)  => e + D2(EX ST 1)Excitation
-5  5  1  1  1  5   1
   6  0  0.0  11.37
     34     1      2.0       9.88e-12      1.47e-8       1.e-6
 -3.081902926338e+01  1.038866780735e+01 -4.259768348687e+00 1.181228673120e+00 -2.277513907465e-01
 2.900576728856e-02 -2.287591474628e-03  1.004346442778e-04 -1.869930069131e-06
*
19. e + D2(GS)  => e + D2(EX ST 2) Excitation
-5  5  1  1  1  5   1
   6  0  0.0  11.7
     34     1      2.0       3.59e-12      1.39e-8       1.e-6
 -3.348199796300e+01  1.371702271009e+01 -5.922607900694e+00 1.709719148860e+00 -3.505232830275e-01
 4.834376067841e-02 -4.131406425550e-03  1.948388368131e-04 -3.854278715563e-06
*
20. e + D2(GS)  => e + D2(EX ST 3) Excitation
-5  5  1  1  1  5    1
   6  0  0.0  12.2
   34     1      3.16       5.27e-12      2.23e-9       1.e-6
-3.646589741675e+01  1.430361969329e+01 -6.074430521073e+00 1.677305768580e+00 -3.128705597349e-01
 3.805424730473e-02 -2.860085821803e-03  1.199641410078e-04 -2.142231851104e-06
```

File Description:

This is the standard Icarus chemistry input file. Formats for different types of reactions (elastic gas, charge exchange, and electron impact) are slightly different however, all reactions follow the same basic input structure. Reaction format: A + B --> (C + E) + (D + F).

First line: Character string (or comment line)

Second line:

entry 1: reaction type (integer)

- 0 elastic gas rxn - kinetic treatment
- -1 charge exchange rxn (fixed cross-section or Janev fit)
- -2 charge exchange rxn using Rapp and Francis relationship
- -3 electron impact rxn
- -4 elastic gas rxn - continuum treatment (for trace-trace chemistry)
- -5 electron excitation reactions (used for electron energy balance)

entry 2: species number for reactant A

entry 3: species number for reactant B

entry 4: stoichiometric coefficient for the first product group

entry 5: stoichiometric coefficient for the second product group

entries 6-9 are the species number of the product species depending of existence

C D or

C E D F or

C D F or

C E D

Third line: (depends on reaction type)

Reaction type 0 or -4: Elastic gas reaction

Arrhenius collisional chemistry reaction rate expression: $k = A\ T^B \exp(-E_a/kT)$

T in K. Requires 5 real numbers:

entry 1 -- number of internal degrees of freedom

entry 2 -- E_a

entry 3 -- A

entry 4 -- B

entry 5 -- heat of rx (+ for exothermic) - joules

Reaction type -1: Charge exchange with cross-section, σ

Requires 2 real numbers:

entry 1 -- cross-section table #; set == 0.0 for constant σ
MUST have a cross-section input table

entry 2 -- σ (m^2) - constant

Reaction type -2: Charge exchange using model from Rapp & Frances(1962)

sigma = (k1 - k2*alog(vr))**2

Requires 4 real numbers:

entry 1 -- k1 for elastic collision

entry 2 -- k2 for elastic collision

entry 3 -- k1 for charge exchange

entry 4 -- k2 for charge exchange

For example, this format was used by Kilgore, Wu and Graves (J. Vac. Sci. Technol. B 12(1)) for an Ar plasma for MKS units on velocity. The following parameter values are given:

7.746x10-10 4.493x10-11 1.288x10-9 7.436x10-11

Reaction type -3 or -6: Electron Impact reactions

Requires 2 integer numbers and 2 real numbers

entry 1 -- equation fit types (if <0, Te in K instead of eV)

Fit 1: K = k1 * (Te**k2) * exp(-k3 / Te)

Fit 2: K = k1 * (Te**k2) * exp(-k3 * Te)

Fit 3: K = k1 * ((k2 / Te) ** k3)

Fit 4: K = k1 * (Te**k2) * exp((k3 / Te) + (k4/Te**2) + (k5/Te**3) + (k6/Te**4))

Fit 5: K = k1 + (Te*k2) + (k3*Te**2) + (k4*Te**3) + (k5*Te**4) + (k6*Te**5)

Fit 6: $\ln K = \sum_{i=1}^{9} k_i \cdot \langle \ln Te \rangle^{i-1}$ (Janev format)

entry 2 -- 0.0 - not used

entry 3 -- heat of formation (e.g., Franck-Condon)- joules

entry 4 -- energy loss per electron reaction - ev

If | fit # | = 1, 2, or 3

input line:

k1, k2, k3

if | fit # | = 4 or 5

input line:

k1, k2, k3, k4, k5, k6

If | fit # | = 6 (Janev format)

first line:

entry 1: reaction # (integer)

entry 2: 1.0 (form of fit - only option at present)

entry 3: min energy to use fit (eV)

entry 4: cross-section at min energy

entry 5: maximun cross-section

entry 6: multiplier to convert cross-section fit result to SI (m**2)

second line:

k1, k2, k3, k4, k5

third line:

k6, k7, k8, k9

Two other example *chem* files follow:

Example 1: A 23 equation set of elastic gas reactions for air chemistry with 5 species: O2, N2, O, N, and NO. Species 1 == O2, 2==N2, etc.

```
*
O2 + N --> 2O + N
0  1    4    2    1    3    3    4
1.           8.197E-19     5.993E-12       -1.         -8.197E-19
*
O2 + NO --> 2O + NO
0  1    5    2    1    3    3    5
1.           8.197E-19     5.993E-12       -1.         -8.197E-19
*
O2 + N2 --> 2O + N2
0  1    2    2    1    3    3    2
1.5          8.197E-19     1.198E-11       -1.         -8.197E-19
*
2O2 --> 2O + O2
0  1    1    2    1    3    3    1
1.5          8.197E-19     5.393E-11       -1.         -8.197E-19
*
O2 + O --> 3O
0  1    3    2    1    3    3    3
1.           8.197E-19     1.498E-10       -1.         -8.197E-19
*
N2 + O --> 2N + O
0  2    3    2    1    4    4    3
0.5          1.561E-18     3.187E-13       -0.5        -1.561E-18
*
N2 + O2--> 2N + O2
0  2    1    2    1    4    4    1
0.5          1.561E-18     3.187E-13       -0.5        -1.561E-18
*
N2 + NO --> 2N + NO
0  2    5    2    1    4    4    5
0.5          1.561E-18     3.187E-13       -0.5        -1.561E-18
*
2N2 --> 2N + N2
0  2    2    2    1    4    4    2
1.           1.561E-18     7.968E-13       -0.5        -1.561E-18
*
N2 +N --> 3N
0  2    4    2    1    4    4    4
1.           1.561E-18      6.9E-8        -1.5        -1.561E-18
*
NO + N2 --> N+O+N2
0  5    2    2    1    4    3    2
1.           1.043E-18     6.59E-10        -1.5        -1.043E-18
*
```

```
NO + O2 --> N+O+O2
0  5    1    2    1    4    3    1
1.           1.043E-18       6.59E-10       -1.5         -1.043E-18
*
NO + NO --> N+O+NO
0  5    5    2    1    4    3    5
1.           1.043E-18       1.318E-8       -1.5         -1.043E-18
*
NO + O --> N + O + O
0  5    3    2    1    4    3    3
1.           1.043E-18       1.318E-8       -1.5         -1.043E-18
*
NO + N --> 2N + O
0  5    4    2    1    4    3    4
1.           1.043E-18       1.318E-8       -1.5         -1.043E-18
*
NO + O --> O2 + N
0  5    3    1    1    1      4
0.           2.719E-19      5.279E-21        1.         -2.719E-19
*
N2 + O --> NO + N
0  2    3    1    1    5     4
0.           5.175E-19      1.120E-16        0.         -5.175E-19
*
O2 + N --> NO + O
0  1    4    1    1    5     3
0.           4.968E-20      1.598E-18        0.5         2.719E-19
*


NO + N --> N2 + O
0  5    4    1    1    2     3
0.           0.             2.49E-17         0.          5.175E-19
*
O+O + M1 --> O2 + M1  (note M1 denotes a third body partner -- the entry of -1 indicates the table in-
dex
0  3    3    1    0    1    0   -1
0.           0.             8.297E-45       -0.5         8.197E-19
*
N+N + M2 --> N2 + M2
*
0  4    4    1    0    2    0   -2
0.           0.             3.0051E-44      -0.5         1.561E-18
*
N + N + N --> N2 + N
0  4    4    1    0    2    0   -3
0.           0.             6.3962E-40      -1.5         1.5637E-18
*
N+O + M3 --> NO + M3
0  4    3    1    0    5    0   -4
0.           0.             2.7846E-40      -1.5         1.043E-18
```

Example *2:* Chlorine plasma with charge exchange and electron impact chemistry

```
**   Chlorine chemistry example -- 11 reaction set
*
*      Cl, Cl+, Cl-, Cl2, Cl2+, SiCl2, e-
*      1     2     3     4     5       6       7
*
*
Cl+ + Cl -> Cl + Cl+ (charge exchange)
-1       2     1      1    1    1    2
       0.75      120.e-20       0.   0.   0.
*
Cl2+ + Cl2 -> Cl2 + Cl2+ (charge exchange)
-1       5     4      1    1    4    5
       0.75     120.e-20       0.   0.   0.
*
*Cl- + Cl -> Cl  + Cl- (charge exchange)
*-1       3     1      1    1    1    3
*        0.90     120.e-20       0.  0.    0.
*
*
Cl+ + Cl- -> Cl + Cl   (recombination)
-4       2    3     1     1     1   1
       0.0    0.0       5.e-14      0.0      1.5e-18
*
Cl2+ + Cl- -> 2Cl + Cl   (recombination)
-4       5    3     2     1     1       1
       0.0    0.0       5.e-14      0.0      1.26e-18
*
*
  Cl2 attachment to Cl + Cl-  (electron impact)
-3       7    4    1   1     1     3
      2   2    5.78e-19   0.0         Franck-Condon
       2.21e-16 0.485 -0.174 0.0 0.0 0.0
*
  Cl- detachment to Cl   (electron impact)
-3       7    3    2   1     7    7    1
       1   1  0.0    3.61
       2.94e-14 0.680 3.7994 0.0 0.0 0.0
*
   Cl2 dissociation to 2Cl  (electron impact)
-3       7    4    2   1     1    7    1
       1   2   0.96e-19    3.12
       3.99e-14 0.115 4.43 0.0 0.0 0.0
*
 Cl2 ionization to Cl2+  (electron impact)
-3       7    4    2   1     7    7    5
       1   1   0.0      11.47
       2.13e-14 0.771 11.7 0.0 0.0 0.0
*
  Cl ionization to Cl+   (electron impact)
```

```
-3      7   1   2  1    7   7   2
        1  1    0.0      12.99
        2.96e-14 0.554 13.1 0.0 0.0 0.0
*
   Cl2+ attachment to 2Cl  (electron impact)
-3      7   5   1  1    1   1
        3   2  1.84e-18     0.0
        9.0e-13 0.0258526 0.61 0.0 0.0 0.0
*
*    electron exicitation reactions -- type -5
*      from E. Meeks 0-D code -- MKS --- T in Kelvin
*
   Cl2 -- vibrational ex.
-5      7   4   1  1    7   4
        -1   1    0.0   0.07Chem.asc (Chemkin file) use:
         2.5141E-08  -1.4443E+00   1.6650E+04   0.0 0.0 0.0
   Cl2 -- electronic ex.
-5      7   4   1  1    7   4
        -1   1    0.0   9.25
         6.3477E-12  -5.3987E-01   1.3920E+05    0.0 0.0 0.0
   Cl -- 4s
-5      7   1   1  1    7   1
        -1   1    0.0   9.55
        1.2363E-11  -6.1356E-01   1.3297E+05     0.0 0.0 0.0
  Cl -- 5s
-5      7   1   1  1    7   1
        -1   1    0.0   10.85
        3.4801E-12  -6.6984E-01   1.4944E+05     0.0 0.0 0.0
  Cl -- 6s
-5      7   1   1  1    7   1
        -1   1    0.0   12.55
        1.9354E-12  -7.3244E-01   1.7005E+05     0.0 0.0 0.0
  Cl -- 3d
-5      7   1   1  1    7   1
        -1   1    0.0   11.65
        9.4444E-11  -7.3093E-01   1.5413E+05     0.0 0.0 0.0
  Cl -- 4d
-5      7   1   1  1    7   1
        -1   1    0.0   12.45
        7.6428E-11  -7.7209E-01   1.6452E+05     0.0 0.0 0.0
  Cl -- 5d
-5      7   1   1 1    7   1
        -1   1    0.0   12.75
        4.7440E-11  -7.8620E-01   1.6810E+05     0.0 0.0 0.0
  Cl -- 4p
-5      7   1   1  1    7   1
        -1   1    0.0   10.85
        1.2295E-10  -8.0133E-01   1.4248E+05     0.0 0.0 0.0
  Cl -- 5p
-5      7   1   1  1    7   1
        -1   1    0.0   12.15
        4.9579E-11  -8.4151E-01   1.5872E+05     0.0 0.0 0.0
```

Chem.asc (Chemkin file) use:

The *chem.asc* file is generated when the Chemkin Interpreter is run. Below is a brief description of the chem.inp file used by the Chemkin Interpreter to generate *chem.asc*, a more detailed description, taken from reference 4 is given in Appendix B. When Init2d is run with a *chem.asc* file it generates a standard Icarus *chem* file (named chem_ck), this allows the user to change the chemistry without having to rerun the Chemkin Interpreter.

Some constraints exist in using Chemkin files for Icarus.

1.) Stoichiometric coefficient of reactants in the chem.inp file must be 1. This will not show up as an error when running the Chemkin Interpreter but is not allowed in Icarus. Init2d will flag this as an error.

2.) Degree's of freedom for all reactions is assumed to be 1.

3.) Reaction type -2 (from Icarus *chem* file) is not allowed when using the Chemkin input file. To add these types of reactions to an existing mechanism that is already in the chemkin format, run Init2d using the chem.asc file and a chem_ck file will be generated. The chem_ck file can be edited and renamed *chem* to include reaction types -2 and then Init2d must be rerun.

4.) Troe parameters or pressure dependent reaction rates are not allowed in Icarus.

There are four sections to a chemkin input file that are indicated by the following key words: **Elements, Species, Thermo,** and **Reactions**. All sections are followed with the word **End**. Comments are any and all characters following as exclamation mark. Details of the format used for the Chemkin Interpreter are found in Appendix B.

Elements contains declaration of all elements contained in any gas phase species.

Species contains all species used in the gas phase mechanism. The format of these species must be the same as the format used in the Icarus *spec* file, Init2d will compare the list of species declared in the *spec* file and compare it to the species found in chem.inp file. **All species in the *spec* file must be declared in the chemkin input file**.

Thermo contains all thermodynamic data for species. This information is not used in Icarus but is required to run the chemkin interpreter. If information in not contained in the input file it must be present in the thermodynamic data base file therm.dat supplied with chemkin. Details of this information can be found in Appendix C.

Reactions contains descriptions of the gas phase reactions, parameters for Arrhenius rate expression ($k = AT^{\beta}\exp^{(-Ea/T)}$), and excitation energies. All reactions, except charge exchange reactions, require the first line of information to include:

reaction description in ASCII textA βEa

Charge exchange reactions (type -1 from *chem*) with constant cross section require slightly different input information:

reaction description in ASCII textprobability $\sigma(m^2)$ 0.0

Auxiliary information is placed on subsequent lines such as excitation energy, temperature dependence (electron temperature dependence for electron impact reactions), etc. The most likely auxiliary key words to be used for Icarus simulations are:

EXCI/ 0.07/ (Excitation energy for the reaction is 0.07 eV)

TDEP/E/ (Specifies that Arrhenius temperature dependence)

DUP (Indicates a duplicate reaction exists in the mechanism, this is typically used for excitation reactions.)

Example 1: Chemkin input file (chem.inp) for a Chlorine plasma chemistry mechanism with Boltzman EEDF to determine rates. This is the same file that was used in Aurora (SNL 0D Plasma code), although charge exchange reactions have been added.

```
ELEMENTS E CL END
SPECIES  E CL+ CL2+ CL-  CL CL2
END
THERMO ALL
300 1000 5000
E               71091E   1    0    0    0G   300.000 10000.000 1000.00    0                1
 0.25002515E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-0.74597845E+03-0.11736856E+02 0.25002515E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-0.74597839E+03-0.11736856E+02                    4
CL              112293CL  1    0    0    0G   300.000  4000.000 1000.00    0                1
 0.29181864E+01-0.35438285E-03 0.12474453E-06-0.20015567E-10 0.11864538E-14      2
 0.13713931E+05 0.32732935E+01 0.23711388E+01 0.96051756E-03 0.23850609E-06      3
-0.20040531E-08 0.11036082E-11 0.13841132E+05 0.60661221E+01                    4
CL*             112293CL  1    0    0    0G   300.000  4000.000 1000.00    0                1
 0.29181864E+01-0.35438285E-03 0.12474453E-06-0.20015567E-10 0.11864538E-14      2
 0.13713931E+05 0.32732935E+01 0.23711388E+01 0.96051756E-03 0.23850609E-06      3
-0.20040531E-08 0.11036082E-11 0.13841132E+05 0.60661221E+01                    4
CL+             112293CL  1E  -1    0    0G   300.000  4000.000 1000.00    0                1
 0.30344462E+01-0.48197978E-03 0.15346743E-06-0.12604539E-10-0.32295198E-15      2
 0.16550063E+06 0.29831080E+01 0.25186882E+01 0.99940156E-03 0.96029623E-07      3
-0.22788400E-08 0.13577272E-11 0.16558978E+06 0.55090742E+01                    4
CL-             112293CL  1E   1    0    0G   300.000  4000.000 1000.00    0                1
 0.25002515E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-0.28878172E+05 0.41883583E+01 0.25002515E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-0.28878168E+05 0.41883578E+01                    4
CL2             112293CL  2    0    0    0G   300.000  4000.000 1000.00    0                1
 0.41252842E+01 0.68196526E-03-0.40838054E-06 0.11656516E-09-0.11435189E-13      2
-0.12794418E+04 0.30671713E+01 0.33467176E+01 0.34548617E-02-0.36136810E-05      3
 0.13227441E-08-0.66440849E-14-0.11213928E+04 0.68718143E+01                    4
CL2+            112293CL  2E  -1    0    0G   300.000  4000.000 1000.00    0                1
 0.41252842E+01 0.68196526E-03-0.40838054E-06 0.11656516E-09-0.11435189E-13      2
```

```
 0.13183581E+06 0.30671713E+01 0.33467176E+01 0.34548617E-02-0.36136810E-05     3
 0.13227441E-08-0.66440849E-14 0.13199384E+06 0.68718143E+01                    4
END
REACTIONS  KELVIN  MOLECULES
! reaction rates from Boltzmann w/ LFA, 50%Cl/50%Cl2, .1% electrons
!      reaction                  A(molecules-cm-s)       b              Ea(K)
 E + CL2  => E + CL2       4.2051E-03           -1.3229E+00   1.0572E+04
  TDEP/E/      !vibrational ex
  EXCI/ 0.07/
  DUP
 E + CL2  => CL- + CL      1.1061E-10   7.3354E-02   2.2957E+03
  TDEP/E/      !dissociative a
 E + CL2  => 2CL + E       4.3770E-10   3.6734E-01   6.1276E+04
  TDEP/E/      !dissociation
 E + CL2  => E + CL2       4.0373E-04  -7.9572E-01   2.3857E+05
  TDEP/E/      !electronic exc
  EXCI/ 9.25/
  DUP
 E + CL2  => CL2+ + 2E     1.7109E-01  -1.0671E+00   3.4343E+05
  TDEP/E/      !ionization
 E + CL-  => CL + 2E       3.3777E-07  -7.1844E-02   8.6257E+04
  TDEP/E/      !detachment
 E + CL  =>  E + CL*       2.2229E-01  -1.3555E+00   2.4567E+05
  TDEP/E/      !4s excitation
 E + CL  =>  E + CL        2.2229E-01  -1.3555E+00   2.4567E+05
  TDEP/E/      !4s excitation
  EXCI/ 9.55/
  DUP
 E + CL  =>  E + CL        1.3323E+01  -1.8428E+00   3.0150E+05
  TDEP/E/      !5s excitation
  EXCI/10.85/
  DUP
 E + CL  =>  E + CL        2.1643E+03  -2.3564E+00   3.6940E+05
  TDEP/E/      !6s excitation
  EXCI/12.55/
  DUP
 E + CL  =>  E + CL        1.4842E+05  -2.4057E+00   3.3453E+05
  TDEP/E/      !3d excitation
  EXCI/11.65/
  DUP
 E + CL  =>  E + CL        1.1564E+06  -2.6237E+00   3.6620E+05
  TDEP/E/      !4d excitation
  EXCI/12.45/
  DUP
 E + CL  =>  E + CL        2.6560E+06  -2.7462E+00   3.7772E+05
  TDEP/E/      !5d excitation
  EXCI/12.75/
  DUP
 E + CL  =>  E + CL        6.8249E+04  -2.4070E+00   3.0212E+05
  TDEP/E/      !4p excitation
  EXCI/10.85/
```

```
  DUP
 E + CL  =>  E + CL        5.4103E+07  -3.0684E+00   3.6520E+05
  TDEP/E/      !5p excitation
  EXCI/12.15/
  DUP
 E + CL  =>  CL+ + 2E      4.2169E+04  -2.1530E+00   3.9624E+05
  TDEP/E/      !ionization
 E + CL*  => CL+ + 2E      2.3983E-07  -2.2218E-02   6.1375E+04
  TDEP/E/      !Cl* ionization
 E + CL*  => CL* + E       2.3983E-07  -2.2218E-02   6.1375E+04
 TDEP/E/      !Cl* ionization energy loss
  EXCI/3.55/
 CL- + CL2+    => CL + CL2        5.00E-08  0.0         0.    !Lee
 CL- + CL+     => 2CL             5.00E-08  0.0         0.    !Bukowski & Lee
! For charge exchange reactions make the first parameter probability, the second parameter cross section.
 CL+  +  CL      => CL + CL+        0.75      120e-20     0.    !CE
 CL2+  +  CL2    => CL2  + CL2+      0.75      120e-20     0.    !CE
END
```

3.10 Diagnostic Messages

The *init2d* code checks for several types of problem areas:

1- length of program arrays
-see section 9.2 for adjusting the parameters in init2d.h

2- region side connectivity
-the code will check the region side connectivity consistency. An error will occur if the region connectivity section is not consistent between two regions

3- files
-the code will provide output to indicate when an input file is opened and closed to facilitate debugging

4- the final screen output from the init2d code contains problem size definition information. This can be used to determine parameters for the param.h file for Icarus, post2d and decomp2d. (section 9.2)

5- Surface boundary conditions are checked to determine if there are sufficient input for each type

6- Warnings are provided when using some of the options. For example, a porous boundary with a porosity of 0.0 (solid wall).

7- The grid is checked in an indirect manner since linear quadrilateral elements are used to determine interpolant and derivative shape functions. Shape errors can occur when the region sides do not conform to the naming convention of init2d.

4.0 decomp2d - Decomposition Code Description

Goal: Decomposes the problem for parallel computing environment.

Usage:**decomp2d** *param1 param2*

param1 and *param2* can be entered either on the command line, as shown, or in response to interactive questions.

param1: number of processors to decompose the input file, datap, into
param2: decomposition strategy (1 for sequential and 2 for block)
(recommend 1 for massively parallel and 2 for few processors)

Input files:
datap: geometry and boundary definition file from **init2d**

Output files:
*dsmc.in2***:** decomposed data file -- specific to # of processors
*dsmc.node***:** link list file to associate cell information with a processor.
used by **restart2d**

Notes:

decomp2d does NOT need to be used if a single processor simulation is being done. The output file from **init2d**, *datap*, can be used directly by **icarus**.

We use decomposition strategy 1 for a tightly coupled computer such as a nCUBE and 2 for other systems: network of workstations, quad-PCs, SGI Power Challenge, IBM parallel systems at LLNL or Maui. .

5.0 icarus - Code and Command File (dsmc.in) Description

Goals: Performs particle move & collisions (DSMC with optional electro-static fields) and gathers statics.

Usage: **icarus** < *dsmc.in*

dsmc.in is a command line redirected input file

Input Files: *dsmc.in2(MP), datap(1P) (file names defined in dsmc.in file)*
dsmc.restart (for restart calculation)
dsmc.plasma, dsmc.power (for icp plasma application)

Output Files: Output filenames are defined in the **dsmc.in**
typical names are: *cell.**, *surf.** , *wafer.**, *chem.**, *plasma.**, *and particle.**.
* denotes the overall time step when file was written (i.e. cell.2000)

File Descriptions:

cell.*	Contains macroscopic quantities of pressure, temperature, density, species concentrations and velocities. Local Cell Knudsen number, CFL number and λ are also contained in this file. An external program, post2d, is used to determine macroscopic properties, determine the type of output variables, and generate a Tecplot formatted plot file.
surface.*	Contains surface element information such as incident flux by species, reflected flux (etchant), surface coverage, surface pressure, shear stress and heat flux. The external program, surface2d, is used to generate a Tecplot formatted plot file.
wafer.*	Contains wafer element information of angular and energy distribution functions by species. The external program, waferxy2d, is used to generate a Tecplot formatted plot file.
chem.*	Contains statistics of the number of times each chemical reaction occurred per cell. The external program, post2d, is used to generate a Tecplot formatted plot of the chemical reaction statistics.
plasma.*	Contains electron number density and temperature for each cell. The external program, post2d, is used to generate a Tecplot formatted plot file of the plasma fields, potential, and local charge density.
particle.*	Contains information on ALL computational particles: position, velocity, species, and kinetic energy
dsmc.log	Contains log information of an Icarus run such as number of time steps, number of particles, number of collisions, number of surface collisions, etc.
dsmc.pump	Contains pump and pressure information when using the pressure feedback loop. Output includes old pressure at control point, new pump speed and current pressure at control point.This file can be used to provide pressure histories at various points during the simulation.

5.1 icarus Command List Summary

This is a complete list of valid DSMC commands found in the *dsmc.in* file, their defaults, and the "type" of parameters that should be used (**i=integer**, **r=real**, **c=character string**). The type (integer, real, character string) of the parameters is important since the input parser expects certain kinds of values. All of the input commands take one or more parameters. The keyword for each command **must** begin in the left most column and all characters in the command must be in lower-case. Parameters can be separated by arbitrary numbers of spaces and/or tabs.

Note: a '*' or '#' as the first character denotes a comment line
typical entries are shown---they may or may not be the defaults

i/o files		
log file	dsmc.log	(c)
id string	character string	(c)
cell file	cell	(c)
surface file	surface	(c)
wafer file	wafer	(c)
movie file	movie	(c)
chemistry file	chem	(c)
plasma file	plasma	(c)
particle file	particle	(c)
pump file	pump	(c)
icp file	icp.out	(c)
directory	name	(c)
problem initialization		
read definition	1.0 dsmc.def	(rc)
read restart	1.0 1.0 dsmc.def dsmc.restart	(rrcc)
read xrestart	1.0 1.0 dsmc.def dsmc.restart	(rrcc)
read efield	dsmc_em	(c)
read plasma	dsmc_plasma	(c)
read power	dsmc_power dsmc_plasma	(cc)
load particles	1.0	(r)
loadn cutoff	0	(i)
loadv cutoff	0	(i)

output control

unformatted	0	(i)
output screen	100	(i)
output cells	0	(i)
output surface	0	(i)
output wafer	0	(i)
output movie	0 0.1	(i)
output chemistry	0	(i)
output plasma	0	(i)
output particles	0	(i)
output fx	0	(i)
ion energy	30.0	(r)
neutral energy	1.0	(r)
species energy	3 20.0	(ir)
output special	50 dsmc.nbari	(ic)

collision/chemistry control

collision flag	1	(i)
chemistry flag	0	(i)
exchange flag	0	(i)
collision limit	5	(i)
secondary electron	0	(i)
coverage	0	(i)
electron chemistry	0	(i)
ereact limit	0	(i)
coulomb	0	(i)
no ionchem	99999	(i)
ion collide	0	(i)

particle injection/gas-surface

surface model	1	(i)
thermal accom	1.0	(r)
BC model	0	(i)
BC ramp	0.0	(r)
inletbc multiplier	1.0	(r)
surface dist	1.0	(r)
voltage bc	0.0	(r)
quasi-neutral bc	1	(i)
target model	1	(i)

dsmc params

adapt flag	50 0.5	(ir)
stat flag	1	(i)
zero flag	100	(i)
random seed	48729873	(i)
statistics	9	(i)

run params

time factor	1.0	(i)
debug flag	0	(i)
limit flag	0 1000.0	(ir)
run	1000 0	(ii)
END		

misc. models

pump speed	1 1.0	(ir)
pump control	1 1.0 0.5 2.0	(irrr)
pump frequency	100	(i)
fx limits	-100. 100. 200	(rri)
fx count	1000.	(r)

plasma options

picflag		1		(i)
ne update		0		(i)
Te update		0		(i)
em update		0		(i)
ap update		0		(i)
ne limit	1.e12	1.e19		(rr)
Te model	1			(i)
Te limits	1.0	10.		(rr)
initial Te	4.0			(r)
constant Te	0			(i)
Te born		1.		(r)
sheath	0.001	0.0	0.0	(rrr)
efield flag		1		(i)
field mult		1.0		(r)
ne mult		1.0		(r)
efield subcycle		1 1		(ii)

e subcycle	1							(i)
ion subcycle	1							(i)
surface charge	0							(i)
volume charge	0							(i)
power model	0							(i)
moving average	10							(i)
charge averaging	1.0							(r)
ne average	0							(i)
ion source	0							(i)
charge regions	4	5	0					(iii)
ambipolar regions	4	5	1					(iii)
charge void	4	5	0					(iii)
charge density	1.e20							(r)
icp flag	0							(i)
ln(lambda)	10.							(r)
charge distance	1.e-6							(r)
ion power	0.0	1.e-5	1.e-5	1	500.	1.e23	10.	(rrrirrr)

5.2 Icarus Command Descriptions

 # comments

blank lines are ignored. Everything on a line after last parameter is ignored. Lines starting with a '*' or '#' are comments and are echoed into the log file.

----------i/o files----------

log file

All info from this point on will dump into this file. Any previous file is closed. New file name can exist, will be overwritten. Anything in input file before the first "log file" command will not be echoed into a log file.
default = none

id string

following character string will be printed at top of output files
default = none

cell file

name of cell file to dump to; timestep # is appended to name. the file can exist--will be overwritten. default = cell

surface file

name of surface file to dump to; timestep # is appended to name. the file can exist--will be overwritten
default = surf

wafer file

name of wafer file to dump to; timestep # is appended to name. the file can exist--will be overwritten
default = wafer

movie file

name of movie file to dump unsteady particle information to; timestep # is appended to name. the file can exist--will be overwritten
default = movie

chemistry file

name of file to write chemical reaction statistics to; timestep # is appended to name. the file can exist--will be overwritten
default = chem

plasma file

name of the file to write plasma properties (electric field vectors, plasma potential, and local charge density) to; time step # is appended to name. the file can exist-will be overwritten
default = plasma

particle file

name of the file to write information on ALL computational particles: position, velocity, species, and kinetic energy. the file can exist--will be overwritten
default = particle

pump file

name of the file to write information about the pump regions and witness points. This file may only contain unsteady pressure at the witness points. the file can exist--will be overwritten
default = pump

icp file

name of the file whose contents is the file name where properties for icp coupled plasma etch systems are computed. this strategy was used to couple the dsmc code for a portion of the simulation and a continuum code for the plasma/electron/electrostatic field simulation.
default = icp.out

directory

name of the directory where files are to be written. by default, the current directory is used. this option may depend on the implementation of MPI for parallel computing
default = none

----------problem initialization----------

read definition

1st parameter = problem size scale factor
2nd parameter = data file

read problem definition from filename (1p from *init2d*; mp file generated by *init2d* & *decomp2d*); use 1st parameter to scale problem size (divides scale base simulation particle scaling computed in init2d input by this value---i.e. >1 increases the number of computational particles); reading a new definition file clears all info from previous runs

read restart

1st parameter = problem size scale factor
2nd parameter = multiplier for initial density
3rd parameter = def data file
4th parameter = restart file

read problem definition from filename and restart info from restart file; restart file is created by running previously generated cell output files thru a serial restart program; use 1st parameter to scale problem size (divides scale base simulation particle scaling computed in init2d input by this value---i.e. >1 increases the number of computational particles); reading a data and restart file clears all info from previous runs; this command causes loading of particles at the cell densities specified in the restart file

read xrestart

1st parameter = problem size scale factor
2nd parameter = multiplier for initial density
3rd parameter = def data file
4th parameter = restart file

same basic definition as 'read restart' except that the cell weights are the values from the definition file (dsmc.in2) rather from the restart file (dsmc.restart). This is useful for subsonic simulations or where the user wishes to have some control on the cell weights.

read efield

1st parameter = efield filename

read efield definition on grid from efield file- values defined at cell corner points. The next "run" following this command must be unsteady. The efield file includes: z(m), r(m), pt. number, E_z and E_r. (file in Tecplot grid format)

read plasma

1st parameter = plasma filename

read plasma values on grid from plasma file- values defined at cell centers. The next "run" following this command must be unsteady. The plasma file includes: z(m), r(m), cell #, Te (eV), and ne.
(file in Tecplot point format - must triangulate before using)
NOTE: this option automatically activates the local ne*te == constant assumption

read power

1st parameter = icp power filename
2nd parameter = continuum simulation file for ne & Te for initial conditions

read icp power values on grid from power file- values defined at cell centers. The next "run" following this command must be unsteady. The power file includes: z(m), r(m), cell #, and ICP power ($J/s/m^3$)
also read initial conditions for the spatial ne and Te -- interpolated to the Icarus grid.
(power file in Tecplot point format - must triangulate before using,
initial conditions in Tecplot format - can use directly)

load particles

initialize cells with particles at initial density and velocity scaled (multiplied) by specified parameter defined in the input file for init2d This command should not be used when a "read restart" command is used, since particles are automatically *loaded* in "read restart". particle properties are obtained by sampling a Maxwellian velocity distribution.
default = 1

loadv cutoff

region with id number <= this number get loaded with particles with initial thermal and velocity components; otherwise only get thermal component of velocity. if = 0, particles in all regions get both initial velocity and thermal components; useful for loading particles in wake region of high-speed flow; NOTE: this input MUST be before the 'load particles' input option.
default = 0

loadn cutoff

region with id number <= this number get loaded with particles at initial density; if = 0, all regions loaded with freestream density; NOTE: this input MUST be before the 'load particles' input option.
default = 0

----------output control----------

unformatted

flag to generate unformatted rather than asci formatted output files. Be careful with moving unformatted files between different computer platforms (e.g., mp machine to compute and a local machine to postprocess); Fortran does not use a standard file description for unformatted files
default = 0

output screen

current timestep info displayed to screen and logfile every this many steps; value of 0 means never display (NOT a wise option)
default = 100

output cells

cell statistics dumped to file every this many steps; always dumped at the end of each run; value of 0 means never dump except at end of run
default = 0

output surface

surface statistics dumped to file every this many steps; always dumped at the end of each run; value of 0 means never dump except at end of run
default = 0

output wafer

wafer statistics dumped to file every this many steps; always dumped at the end of each run if wafer material type is defined through init2d input; value of 0 means never dump except at end of run
default = 0

output movie

1st parameter = every this many steps
2nd parameter = probability of tagging a particle

particle stats dumped to movie file every this many steps; also dumped at the end of each run; 2nd param determines what fraction of current particles are written to file; currently this command only works if are running on 1 processor; value of 0 means never write info.
default = 0

output chemistry

chemical reaction statistics are dumped to file every this many steps; always dumped at the end of each run if chemistry flag is on; value of 0 means never dump except at end of run
default = 0

output plasma

plasma parameters are dumped to file every this many steps, contains ne and Te. Values are either initial values or updated ne based on local charge neutrality assumption. Used to verify plasma parameters used for computing electron impact chemistry rates. Also, the electrostatic fields and either plasma potentials (volts) or power (watts) are output (if electrostatic fields are determined, potentials are used).
default = 0

output particles

computational particle information (position, velocity, species type, kinetic energy) are dumped to a file every this many steps. this option is both 1p and mp enabled.
default = 0

output fx

option in the logic to obtain velocity distributions a various cell locations (defined via init2d). This option is used to SKIP this many time steps BEFORE accumulating statistics. this allows the initial, assumed distributions to be relaxed.
default = 10000000000

ion energy

maximum value (in eV) to scale ion particle energies for the wafer (incident angular and energy distributions). see also *species energy* command.
default = 30.0

neutral energy

maximum value (in eV) to scale neutral particle energies for the wafer (incident angular and energy distributions). see also *species energy* command.
default = 1.0

species energy

1st parameter = species id number
2nd parameter = energy value (eV)

set the maximum particle energy for this species in the *wafer* logic (incident angular and energy distributions). this command overrides those defaults for a specific species via either *ion energy* or *neutral energy*; energy value of 0.0 unsets a previous setting.

output special

1st parameter = frequency of obtaining output
2nd parameter = file name. time step appended to name at time of creation.

This is a special purpose, user modifiable, output section. As provided in Icarus, the routine (located in output.f) will automatically average the densities (by species) across all cells and output a single value. This was used to increase the statistics when simulating 0D effects such as vibrational relaxation on a multi-processor computer; each processor can be running its own problem (with its own random seed) and the results averaged.

----------collision/chemistry control----------

collision flag

flag for whether or not to perform elastic, particle collisions:
0 = do not, 1 = do collisions.
If flag is set to 0, there can obviously be no chemical reactions unless the continuum chemistry formulation is used.
default = 1

chemistry flag

flag for whether or not to perform particle chemistry:
0 = no chemistry, 1 = particle chemistry using steric factors or electron chemistry using reaction rates
default = 0

exchange flag

flag for kind of energy exchange during particle collisions:
0 = Borgnakke-Larsen, 1 = not implemented at this time
default = 0

collision limit

max number of particle collisions allowed for any one particle during a time step. greater than about 4 or 5 will not change the energy partitioning as the particles are simply moving about the Maxwellian. However, this option should not be used when particle chemistry is on since the effective rates will be lowered.
default = 5

secondary electron

flag to determine if secondary electrons should be created during electron chemistry.
0 = do not create, 1 = create
this option is typically used (= 0) when performing a simulation using ambipolar fields based on local charge neutrality; electron motion is not simulated via particles. Note that secondary electron emission from surfaces are controlled in the surfbc file.
default = 1

coverage

Number of time steps between updating the available surface sites for the coverage chemistry calculation during the unsteady portion--Note: coverage chemistry activated by input files (chemistry) from **init2d**
default=500

electron chemistry

option when simulating multiple electron species (e.g. e- and e- with increased mass) to specify the species number to used for electron chemistry
0 = code determines from input files (last electron found is used), >0 = specifies species #
default = 0

coulomb

flag to determine if coulomb cross-section should be used instead of VHS/VSS for interactions between charged particles; a simple Spitzer model is used (see ln(lambda) input option)
0 = do not use model, 1 = use model
default = 0

no ionchem

option to turn off Lorentz force transport and electron impact chemistry for regions greater than or equal to this value
default = 99999 (operate in all regions)

ion collide

option to turn off elastic (including coulomb) collisions for the ions.
0 = no collisions, 1 = collisions;
recombination chemistry can still occur if chemistry option '-4' is used (continuum chemistry)
default = 1 (ion collisions)

----------particle injection/gas-surface----------

surface model

model determines the mean energy of the diffuse surface reflected particles.

0 = mean energy is probabilistically determined based on the thermal accommodation coeff. - either the incident (specular) or surface (diffuse) energy.

1 = energy is a deterministic weighted sum between the incident and surface energy based on the thermal accommodation coeff. (this option and *thermal accom 1.0* is the traditional DSMC surface interaction)

default = 1

thermal accom

gas-surface thermal accommodation factor--overrides the input value from the initialization files. Must appear after the "read def" command since the value is set to 1.0 or user input via init2d.

default = 1.0

BC model

This controls various initial velocity distribution models for inflow boundaries on surfaces:

0 - V-normal = sample from a drifted Maxwellian
V-parallel = superposition of thermal Maxwellian + specified mean

1 - V-normal = specified mean
V-parallel = specified mean

2 - V-normal = specified mean
V-parallel = superposition of thermal Maxwellian + specified mean

3 - V-normal = superposition of thermal Maxwellian + specified mean
V-parallel = superposition of thermal Maxwellian + specified mean

4 - sample from input distribution -- see routine *distbc*

default = 0

BC ramp

input is the time over which the inlet flux is linearly ramped to its constant value

default = 0.0

inletbc multiplier

multiplies the inlet boundary fluxes. This option alleviates the requirement to re-run init2d to evaluate the system response to different boundary fluxes.

default = 1.0

surface dist

the power of the cosine distribution to obtain the thermal spread of the inlet boundary particles.

default = 1.0

voltage bc

input to override the base potential from a electro-statics surface with BC type 5 to allow system responses to be determined without re-running the init2d code. See option *target model* to determine how the surface potential in the domain is computed

default = 0.0

quasi-neutral bc

models to determine the inlet flux of electrons to obtain a local, quasi-neutral plasma.

0- no model - electron flux specified via inlet definition in init2d

1- assume a Child-Langmuir surface (not recommended)

2- inject sufficient electrons to identically obtain a quasi-neutral plasma in the injection cell (recommended). Note that the electrons will be injected with the velocities (energy) from the surface file; the flux will be determined to obtain a charge neutral boundary cell.

default = 0

target model

models to determine the time varying electro-static potential on a surface

1- simple circuit to a given potential: single resistance. potential determined from voltage drop with the incident ion/electron flux (current) and resistance

default = 1

----------dsmc params----------

adapt flag

adjusts cell weight to reduce # of computational particles/cell; *mass is conserved*
1st parameter = number of particles per cell to limit to
2nd parameter = tolerance factor (delete particles if more than n*(1+tolerance))
for efficiency of adapt routine, tolerance should be set >= 0.25
default = 50 0.5

stat flag

accumulate cell statistics every this many timesteps; 0 = never accumulate
default = 1 (every step)

zero flag

zero out accumulation quantities every this many timesteps; used to run unsteady flow to estimate the local macroscopic properties; is ignored when running steady flow; 0 = never zero out quantities
default = 100

random seed

initial seed for random number generator
default = 123456789

statistics

the length of the statics array in use (< dimension gmstat). This is used to control the amount of data in the cell.* output files. A value of 9 captures the typical moments from a 2D simulation
default = 9

----------run params----------

time factor

time scale factor to multiply timestep by in all regions; this parameter is NOT cumulative; should be set explicitly to the desired scale factor to dilate or compress time for each stage of a run. for example, one can set the default time step in init2d to 1.e-6 and simply modify that in this file.
default = 1.0

debug flag

flag for whether to print verbose messages to screen
0 = none,
-5 = output the element surface charge from the Poisson solver (diagnostic purposes)
-2 = debug and timing info in the Poisson solver and output element charge at t=0
-1 = definition file printout checkpoints
1 = some (hung particles in move),
2 = debug info during move
3 = module debug info (in dsmc)
default = 0

limit flag

1st parameter = # of timesteps
2nd parameter = # of CPU seconds
check every this many timesteps to see if total run time has exceeded this many CPU seconds; value of 0 for 1st parameter means never check; if it has, stop the program immediately
default = 0 for 1st parameter (do not check run time)

run

1st parameter = # of timesteps
2nd parameter = 0 (unsteady). 1 (steady)
run or continue DSMC for this many timesteps.
unsteady mode: zeroes out cell, surface, and collision statistics at the beginning of the "run" command and every so many steps (see "zero flag" command). Also resets the maximum σV_r per cell used by the NTC collision model.
steady mode: all statistical quantities continuously accumulate

END

will terminate program execution and close opened files.

----------misc. models----------

pump speed

1st parameter = pump region

2nd parameter = pumping speed (in m^3/sec) {value of 0.0 turns off pump}

The pump model is a self-consistent strategy to obtain a constant volume outflow boundary condition, e.g. a vacuum pump.

default = 0.0 for all regions

pump control

1st parameter = pump region

2nd parameter = target pressure in specified cell (Pascals)

3rd parameter = minimum allowed pump speed

4th parameter = maximum allowed pump speed

control pump speed so as to achieve target pressure in one simulation cell; this command only applies to the next “run”, which must be unsteady; cell # for target pressure is specified in “read definition” file; initial pump speed will be whatever is specified by “pump speed” command; pump speed will be kept between min and max values.This model is a strategy to obtain a constant pressure boundary condition in the DSMC code.

pump frequency

frequency to compute the witness point pressure and to adjust the pumping speed if feedback monitoring is in effect

default = 100

fx limits

1st parameter = minimum velocity

2nd parameter = max. velocity

3rd parameter = number of distribution bins (< 400)

This option, in conjunction with *fx count* and *output fx*, are used to obtain the velocity distributions for V1 and V2 at the ’pump’ witness points.

fx count

The number of samples at each witness point before the distribution is outputted. A separate file is generated for Fv1 and Fv2 for each witness point.

----------plasma options----------

picflag

flag to determine whether the average charge density or the instantaneous particle charge will be used to determine the electrostatic plasma potential.

0 average quantity (either discrete average (DSMC) or moving)

1 instantaneous

default = 0

ne update

flag to invoke local charge neutrality for calculation of ne (electron number density). Perform averaging every ne update global (neutral) time steps in both unsteady and steady phases. The local Te is updated assuming a local neTe==constant (constant updated via Te update). The space charge electric field update (Boltzmann distribution) is called with the new ne.

default = 0

Te update

global (neutral) time step frequency to update Te based on an electron energy balance. A local cell energy balance (neTe = constant) is used for the other time steps after an ne update.

default = 0

em update

time step frequency to update the electro-static fields (either by Poisson or ambipolar assumptions). Non-physical oscillations may occur if > 1 (particles move too far before the local space charge fields are updated).

default = 1

ap update

time step frequency to update the electo-static fields using an ambipolar assumption (Langmuir-Tonks) in a *mixed field problem*. That is where the fields in a portion of the domain are determined by a Poisson equation and a portion by an ambipolar assumption. (see the tube sample problem)

default = 0

ne limit

minimum and maximum values for electron number density (ne) based on local charge neutrality

default = 1.e12 and 1.e19 #/m3

Te model

which model is used to determine the cell averaged electron temperature.

1 a control volume approach is used to solve a continuum-like electron energy equation for Te. Electron excitation and electron chemistry heat of reaction, ohmic heating, and conduction effects are included

2 a quasi-kinetic approach is used

3 the average electron temperature is based on the average electron kinetic energy

default = 1

Te limit

minimum and maximum values for electron temperature (Te) assuming a Boltzmann distribution.

default = 1.0 and 10.0 eV

initial Te

initial (t = 0.0) electron temperature (Te), assuming a Boltzmann distribution.

default = 0.01 eV

constant Te

flag to not update Te -- to force Te(i,j) to be constant in time.

default = 0

Te born

the temperature (eV) when electrons are created during an electron-impact event

default = 0.1

sheath

sheath parameters for the bulk plasma/sheath model

1st parameter = sheath thickness (m)

2nd parameter = voltage drop in sheath which is NOT wafer

3rd parameter = voltage drop in wafer sheath

defaults = 0.001 0.0 0.0

efield flag

various strategies to compute or obtain electro-static fields

0 = no fields (turn them off if used previously)

1 = use external fields (see *read efield*)

2 = use internally generated space charge fields - Langmuir-Tonks (ambipolar) model

3= do both 1 & 2 as a superposition of fields

4= use a Poisson Green's function solver

5 = no fields but can have plasma chemistry (usually for testing)

6 = mixed: use Poisson for a portion of domain and ambipolar for portions

if 1 or 3 is specified then you must do a *read efield* before unsteady "run"

default = 0

field mult

multiply the electrostatic fields by this value; must occur BEFORE the *read efield* command to alter the input values.
default = 1.0

ne mult

multiplier for the input electron number density - must occur BEFORE the *read efield* command
default = 1.0

efield subcycle

1st parameter = # of timestep subcycles in bulk interior region

2nd parameter = # of timestep subcycles in sheath region

number of timestep subcycle to perform in particle move of charged ions only useful when "efield flag" is set so as to turn on efields

default = 1 1

e subcycle

option to allow electron time step frequency to be an integer multiple of the ion time step frequency. During an electron subcycle time step, only the electrons will move; however, a general collisional step is performed with all particles (which can create/destroy electrons)
default = 1 (same time step for electrons and ions)

ion subcycle

option to allow ion time step frequency to be an integer multiple of the neutral time step frequency. During an ion subcycle time step, only the ions will move; however, a general collisional step is performed with all particles (which can create/destroy ions)
default = 1 (same time step for ions and neutrals)

surface charge

set this flag to 1 to include the surface charge in the Poisson electro-static field solver (only on dielectric surfaces). not fully implemented
default = 0 (do not include surface charge)

volume charge

used to control regions where the cell charge should be included in the Poisson electro-static field solution and also regions which will not have a cell potential determined. useful for domains with Poisson and ambipolar (charge neutral) regions.

1st parameter	beginning region #
2nd parameter	ending region #
3rd parameter	flag (0 - exclude, 1 - include)

default = 1 (include volume charge)

power model

1 normalize icp power (J/s) by sqrt(local electron number density)
default = 0

moving average

model determines the average local charge density by a true moving or sliding average as contrasted by using the traditional DSMC incremental averaging scheme. Input is the width of the window (< 50). This window is incremented based on the frequency which the Poisson solver is called which may be less than or equal to the global particle move time step(see emupdate). The following option turns on this option.
default = 30

charge averaging

control type of charge averaging
0.0 <= value <= 1.0 backward time averaging (1.0 = current time, no time averaging)
<0 use moving average scheme
default = 1.0

ne average

0 use instantaneous local charge neutrality to compute ne
1 time average old + instantaneous
default = 0

ion source

flag used for simulations of ion accelerators; computes the inlet ion current to ratio the target current. (1 set flag, 0 off)
default = 0

charge regions

used to control regions where the cell or volume charge should be excluded in determining the spatial potentials in the Poisson electro-static field solution.
1st parameter beginning region #
2nd parameter ending region #
3rd parameter flag (0 - include, 1 - exclude)
default = 0 (include volume charge)

ambipolar regions

used to define regions where local charge neutrality and ambipolar electrostatic fields are assumed in a mix ambipolar and Poisson solver simulation
1st parameter beginning region #
2nd parameter ending region #
3rd parameter flag (0 - off, 1 - on)
default = 0 (no ambipolar fields)

charge void

used to define regions where there is no charge density; typically non-plasma regions

1st parameter	beginning region #
2nd parameter	ending region #
3rd parameter	flag (0 - none, 1 - charge)

default = 1 (all charge regions)

charge density

if > 0.0, domain has constant charge density at this value (#/m^3)
default = 0.0

icp flag

frequency to check for updated ICP power file in a coupled DSMC and external power deposition code iteration scheme.
default = 0

ln(lambda)

log lambda value used in the Spitzer coulomb collision cross-section model
default = 10.

charge distance

maximum radius to use in the volume integral computation for the electro-static potential
default = 200.e-6 (m)

ion power

model to approximate the plasma power deposition from an arc discharge. (only implemented in axisymmetric coordinate system). model assumes a cylindrical power deposition volume

1st parameter	in z coordinate of power cylinder
2nd parameter	max z coordinate of power cylinder
3rd parameter	radius of cylinder
4th parameter	region where power deposition is located
5th parameter	source power (watts)
6th parameter	initial electron density to initiate discharge
7th parameter	initial electron temperature (eV)

5.3 Example dsmc.in Files

Example 1: Using Initial Freestream Conditions

```
# Neutral flow reactor dsmc.in file

log file             dsmc.log
output screen          100
zero flag            100
pump control           1   0.75 0.003 0.3
pump speed             1   0.03
pump file               dsmc.pump
pump frequency       100
read definition        0.2  dsmc.in2
load particles         6.0
adapt flag           500 0.25
time factor            1.0
run                20000 0
output cells           5000
output surface         5000
adapt flag           1000 0.25
time factor            1.0
run                400000 1
```

Example 2:Using Restart File

```
#shield calculations with shorter length

log file             dsmc.log
output screen          100
zero flag            100
pump control           1   0.75 0.003 0.3
pump speed             1   0.03
pump file               dsmc.pump
pump frequency       100
read restart           1.0  0.3 dsmc.in2 dsmc.restart
adapt flag           500 0.25
```

```
time factor          1.0
run                 20000 0
output cells         5000
output surface       5000
output wafer         5000
adapt flag          1000 0.25
time factor          1.0
run                400000 1
```

5.4 Diagnostic Messages

1- code parameters are checked with input values...see section 9.2 for changing param.h

2- if the ‘debug flag’ is set to -1, input diagnostic as the file is read will be performed

3- messages: ‘Too many in reacta’ or ‘Too many in create’ indicate that the max. number of particles per processor has been exceeded (lmmo in param.h). Either increase lmmo and recompile or use the adapt flag to limit the number of computational particles per cell.

4- a message: ‘Too many in self-communicate’ indicates that the communication buffer array is too small (gbuf in param.h). Either increase gbuf and recompile, decrease the time step, or limit the number of particles in the simulation by using the adapt limit or the global scale factor on the *read def* (*read restart*) input.

5- ‘Stop - Comm buffer overflow’ indicates that the buffer is too small....code hangs in a MP environment. Either increase the buffer size, gbuf, and recompile or reduce the number of simulation particles by using adapt or the global scale factor on the *read def* (*read restart*) input.

6- Icarus checks for consistency between the input files (dsmc.in2 and dsmc.restart) and the number of processors requested. That is, you cannot run a 2 processor simulation if either the input file, dsmc.in2, or the restart file, dsmc.restart, were created for a different number of processors or load balancing schemes. Rerun either (or both) *init2d* or *decomp2d* as necessary.

7- a message in “which surface” indicates that a computational particle is *hung.* That is, round-off error has caused a particle position to be undefined in the computational domain. This error is only a problem if it occurs many times per time step; check the output after a run step (unsteady or steady) where the #-hung particles per time step are computed. If debug flag is on, then

hung 1 = particle moved to another region and lost

hung 3 = too many bounces (> maxk)

hung 4 = particle hits surface and lost

8- Check the output after each run step (unsteady or steady) for global statistics to determine if the simulation is running satisfactory. For example, for statistical reasons, there should be at least ~10 particles per cell.

9- Load balancing information is printed at the end of each run step (unsteady or steady). This information includes a 10 group histogram of the computational time during specific code blocks.

10- messages: ‘Too many in init’ or ‘Too many in create’ indicate that the max. number of particles per processor has been exceeded (lmmo in param.h). Either increase lmmo and recompile or use the adapt flag to limit the number of computational particles per cell. NOTE: when this message occurs, no more computational particles are loaded into the cells for that processor. For example, during problem initiation, if the message: ‘Too many in init’ occurs, then the remainder of the cells for that processor will not have any particles -- a vacuum condition.

6.0 restart2d - Code Description

Goal:Generate starting solution for a icarus calculation with the same grid.

Usage:**restart2d** *cell.* value*

*cell.**: **icarus** cell data file (default *cell.1000, cell.2000,* etc.)
value: optional input: 2 for a mp restart case and 1 for a single processor case
Note: if *dsmc.node* file (mp file) does not exist, single processor assumed
interactive response to creation of a mp(2) or single processor(1) restart file

Additional Input files:
if single processor file, none
if mp restart file, *dsmc.node* (from **decomp2d**)

Output files:
dsmc.restart: file for **icarus**

Notes:

mp to mp

The dsmc.node file has to be decomposed for the restart calculation (*dsmc.in2*). You can change the number of processors between restart runs(i.e. start with 256 and then restart with 128).

1p to mp

Just use the *dsmc.node* file of the decomposed input file.

mp to 1p

Just select the option, 1, to decompose into a *dsmc.restart* file for a 1p simulation.

misc:

restart2d only requires the number of grid cells and region distribution to remain the same as well as the number of chemical species; boundary conditions, reaction rates, vacuum pump flows, etc. can be changed during the restart simulation.

NOTE: *restart2d* uses only the macroscopic properties (cell density, velocity, temperature, etc) and assumes a Boltzmann distribution to restart a simulation. Therefore, several unsteady time steps are required to obtain non-equilibrium conditions before the steady ensemble

phase should begin.

7.0 regrid2d - Code Description

Regrid2d takes an existing output cell file from Icarus and will interpolate it onto a new mesh system. This is different than restart2d which simply takes an output cell file from Icarus and creates a restart file for the same grid system. Regrid2d uses a 5 point weighted least squares method; therefore, it is a robust strategy when changing grid schemes but is computationally extensive. Restart2d is much faster than regrid2d and should be used if possible. Both methods assume that the restart flow field will be created from sampling a Maxwellian based on mean properties from either a regrid2d or restart2d file.

usage: regrid filex

input file - filex: a cell.x file from an existing Icarus simulation

assumed files:

datap_old	datap from the existing or old Icarus grid system
dsmc.in2	file for new grid (decomp2d has been run)
dsmc.node	decomposition strategy for new grid if not there---a single processor is assumed

output file:

dsmc.restart	restart file for Icarus (either 1p or mp depending on dsmc.node)

8.0 Postprocessing Codes

post2d:

-cellwise information
-converts particle statistics into macroscopic quantities:
pressure, density, velocities, temperatures, species concentrations, etc.
-use cell data files from icarus

surface2d:

-information for surface elements (sides of cells which are boundaries):
surface pressure, shear stress, & heat flux
-incident flux by species
-reflected flux from surface reactions (i.e. etch products)
-use surface cell files from icarus

waferxy2d:

-angular and energy distribution of incident particles (by species)
-information only for designated surfaces (storage limitations)
-output format is in pseudo-2D format
-use wafer files from icarus

stat2d:

-generate statistics between two output files (different iteration steps)
-quantify the rate of change of specific variables to indicate whether a converged solution has been attained.
-NOT CURRENTLY OPERATIONAL FOR NEW TECPLOT BINARY FORMAT

example usage:
post2d *cell.10000 file2*
(file *cell.10000* from icarus, file *file2* created by post2d)

preplot *file2*
(Tecplot supplied file to create binary input file *file2.plt*)

tecplot *file2.plt*
(Tecplot graphics package for *file2.plt* data set)

Default output file format is Tecplot (commercial plotting package)

8.1 Macroscopic Cell Information (post2d)

Goal:-specify the output variables from the cell data file
-re-order spatial coordinates
-units conversion (i.e. pascals to mtorr, K to C, meters to cm or inches)

Usage: **post2d** *arg1 arg2 arg3 arg4*

arg1: filename (cell.xx, chem.xx, or plasma.xx) or
if == 'pr', output list of variable option (requires datap file)
arg2: output filename (default == 'ffout')
arg3: if 'u' or 'U', cell.xxx file in unformated structure
arg4: grid data file (default = 'datap')

examples:

post2d *cell.* cellout*
see post2d.vlist description for available cell information
or **post2d** *chem.* chemout*
cell reaction statistics (by each reaction)
or **post2d** *plasma.* plasmaout*
plasma characteristics: electrostatic fields, potential, charge density

cell.:*output data file from **icarus** code -- for example *cell.40000*
*cellout:*output file in Tecplot format (requires preplot)

post2d.vlist:control file read by post2d to specify the output variables and multiply values for optional unit conversion for a cell.xx file. The cell file contains a vast amount of information; post2d.vlist controls the *data mining* into this file. If the multiplier is -999., then the log (base 10) is taken of the data (this is useful when there are orders of magnitude variations in a variable such as density in the domain).

Variables:-variables 1 - 24 are default in the *cell.** file (hardwired Variable Index number)
-'*' in column 1 signifies a comment

Variable TypeVariable Name

1 X or Z (first dimension-m)
2 Y or R (second dimension-m)
3 #/cell (average number of computational particles per cell)
4 number density (#/m3)
5 pressure (pascals)
6 cell weight (Icarus parameter)
7 velocity, first direction - Vx or Vz (m/s)
8 velocity, second direction - Vy or Vr (m/s)
9 Maxwellian translation temperature (K)
10 rotational temperature (K)
11 vibrational temperature (K)
12 overall temperature (K) - weighted by DOF
13 cell CFL number (avg. velocity / cell length/dt)
14 Mean Free Path MFP (m)
15 local Knudsen number based on density gradient length
16 cell Knudsen number - s13 (mfp / cell side 1)
17 cell Knudsen number - s24 (mfp / cell side 2)
18 $\log_{10}$ (number density)
19 $\log_{10}$ (pressure)
20 average # computational particle collisions in cell
21 average cell side (1 & 3)
22 average cell side (2 &)

if plasma option

23 charge neutral electron number density
24 neutral number density

5x species x mole fraction
10x species x velocity for first dimension (m/s)
20x species x velocity for second dimension (m/s)
30x species x average translational temperature (K)
40x species x average translational temperature (K) - direction 1 (x or z)
50x species x average translational temperature (K) - direction 2 (y or r)
60x species x rotational temperature (K)
70x species x vibrational temperature (K)

Note: use the string, 'END', as the last variable name to avoid problems with extra lines at the end of the file.

Example *post2d.vlist* file

```
*
*   * in col 1 for comment or to comment out a line
*     specie number fractions are 5x where x is the specie #
*     specie velocities are in pairs of 10x and 20x for Vz and Vr
*
*Var. name(10 Char MAX)     multi. factor     Var. index
X(m)                        1.                1
Y(m)                        1.                2
n                           1.                4
p(mtorr)                    7.50075           5     convert Pa to mtorr
Vx(m/s)                     1.                7
Vy(m/s)                     1.                8
Tt(k)                       1.                9
Kn                          1.                13
CFL                         1.                14
Ar                          1.                51    species mole fract. inputs
N2                          1.                52
Ti                          1.                53
*N                          1.                54
*Ar+                        1.                55
*Sih4                       1.                55
Vx_Ar                       1.                101    species Velocities
Vy_Ar                       1.                201
Vx_N2                       1.                102
Vy_N2                       1.                202
*Vx_Ti                      1.                103
*Vy_Ti                      1.                203
*Vx_N                       1.                104
*Vy_N                       1.                204
*Vx_Ar+                     1.                105
*Vy_Ar+                     1.                205
t Ar                        1.0               301    species temps.
t N2                        1.0               302    species temps.
t Ti                        1.0               303    species temps.
END
```

8.2 Surface Information (surface2d)

Goal: Converts boundary cell information to surface fluxes and reactant fluxes (etchant flux).

Usage:**surface2d** *arg1 arg2 arg3 arg4 arg5 arg6*

arg1: input file (surface.xx from Icarus)
arg2: output file name
arg3: if 'u' or 'U', file in unformatted mode
arg4: number of regions to extract surface data for
arg5: region numbers
arg6: surface material number to limit data mining

example: surface2d surf.100 surf100 x 2 1 3 4
(2 regions (3 & 4), material 4)

(note: region #'s to plot and material #s from *geometry.inp* file)

Other Input Files:
datap

Variables:

1	X or Z	first dimension, X or Z (m)
2	Y or R	second dimension, Y or R (m)
3	P	surface pressure (pascals)
4	shear	surface shear stress (N/m^2)
5	qwall	surface heat flux (W/m^2)
6	avg. hits	average number of particle-surface collisions per time step
7	tot. hits	total number of particle-surface collision in sample
7+1	I spec1	incident flux for species 1 ($\#/m^2$-s)
7+2	I spec2	incident flux for species 2 ($\#/m^2$-s)
7+i+1	R spec1	surface reaction flux for species 1 (#/m^2-s)
7+i+2	R spec2	surface reaction flux for species 2 (#/m^2-s)

Note: spec1 and spec2 will be replaced with their respective character strings from the *spec* file.

8.3 Wafer Information (waferxy2d)

Goal: Convert boundary wafer cell statistics to incident angular and energy distributions.

Usage:**waferxy2d** *wafer.** *waferout*

*wafer.** from **icarus** code (i.e. wafer.1000)
waferout in Tecplot format
(the surface cells designated as 'wafer' are defined in the *geometry.inp* file.)

Other Input Files:

datap

Variables:1first dimension, X or Z (m)
2 second dimension, Y or R (m)
3 delta angle increment, dAng (deg)

4 normalized angular distribution function for species 1 (A spec1)
5 normalized angular distribution function for species 2 (A spec2)
.
.
3+i normalized angular distribution function for species i (A speci)

3+i+1 delta energy increment for species 1, del1 (eV) (dE spec1)
3+i+2 normalized energy distribution function for species i, eng1 (E spec1)
.
.

note: spec1, spec2, and speci will be replaced with their respective character strings from *spec* file

to plot normalized angular distributions:
select variable 3 for the x plot variable
select variable 4 - 3+i for the y plot variable

to plot normalized energy distributions:

select variable 3+i+1 for the x plot variable for species 1
select variable 3+i+2 for the y plot variable for species 1

Note: The reason for this data structure is that all species have the same angular increment for

the angular distribution function (1 degree for axisymmetric systems and 2 degrees for cartesian).

However, each species can have its own range of energy distribution function: 0 to X ev.

The output data is normalized by species for both the angular and energy distributions.

8.4 Cell Convergence Statistics (stat2d)

NOT CURRENTLY OPERATIONAL FOR CURRENT TECPLOT BINARY FORMAT

Usage: **stat2d** *cell.** *cell.***

*cell.**: 2d tecplot binary of dsmc solution at time 1
*cell.***: 2d tecplot binary of dsmc solution at time 2

the order of file1 and file2 is not important.

Other input files:
post2d.vlist: for each variable in column 3 (third variable after variable name)
0- skip variable
1- obtain statistics for variable
note: is standard default post2d.vlist is used, no variables are marked

Output files:
stat.out - A text file with following info for each region and globally.
min(%) = percent change in the min value of a variable between solution planes.
max(%) = percent change in the max value of a variable between solution planes.
mean(%) = mean percent change in a variable between solution planes.
standard deviation = the standard deviation of the change in a variable between solution time planes.

stat.tec - A text file which can be read into tecplot. The stat.tec file allows the min(%), max(%), mean(%) and standard deviation of a variable to be plotted versus region number.

9.0 Install/Compile Software

9.1 Make files

The Icarus code and the utilities are in a directory structure under the directory, icarus.

./icarus/code-	source code for Icarus (DSMC)
./icarus/code/util-	source codes for utility programs: init2d, post2d,....
./icarus/samples -	sample problem files (see appendix B)
./icarus/documentation -	pdf file of this document

To compile the Icarus (DSMC) code:

note: the Blas library is used in the Poisson solver routine. Machine compiled libraries are available for Windows using the Absoft (mkl_c.lib) or Visual Fortran Compilers (mkl_s.lib). The source for Blas is provided if case local versions of blas.lib are not available. If electro-static fields computed using a Poisson solver are not required, one can simply comment out the calls to the Blas routines found in poisson.f

cd ./icarus/code

make help (to see the various options)

```
$ make help
Type "make target" where target is one of:
aixmp     (for IBM SP with ppe/poe)
 ncube     (for nCUBE-2 w/MPI)
ncubeg    (for nCUBE-2 w/MPI -g option)
 mos       (for Intel Paragon w/ SUNMOS MPI)
 tflop     (for Intel Tflop w/ MPI)
 pcmpi      (for PC/NT w/MPI - Dec Fortran)
pcmpig     (for PC/NT w/MPI: -g -C Dec Fortran)
 pc        (for PC/NT 1p - Absoft)
 pcg       (for PC/NT 1p  -g -C option - Absoft)
pcg2       (for PC/NT 1p  -g    option - Absoft)
 pcdec      (for PC/NT 1p - Dec Fortran)
pcdecg     (for PC/NT 1p: -g -C option Dec Fortran)
sun       (for Sun 1p)
sung       (for Sun 1p w/ -g -C option)
sunmpi     (for Sun w/MPI)
sunmpig    (for Sun w/MPI w/-g option)
```

To install the utility codes:

cd ./icarus/code/util

for UNIX systems:

make sunV (for SUN Solaris)
or
make sunos (for SUN SUNOS)
or
make sgi (for SGI)
or
make hp (for HP)
or
make ibm (for IBM RS6000)

for PCs, for each package (init2d, decomp2d, post2d, surface2d, etc)

make -f makepc init2d --- uses the Absoft Fortran compiler
make -f makepc init2dg --- uses te Absoft Fortran compiler - debug option
make -f makepc init2ddec --- uses the Visual Fortran compiler
make -f makepc init2ddecg -- uses the Visual Fortran compiler - debug option
make -f makepc post2d --- uses the Absoft Fortran compiler
make -f makepc post2ddec -- uses the Fisual Fortran compiler
make -f makepc restart2d -- uses the Absoft Fortran compiler
make -f makepc restart2ddec -uses the Visual Fortran compiler
make -f makepc regrid -- uses the Absoft Fortran compiler
make -f makepc reggriddec -- uses the Visual Fortran compiler
make -f makepc surface2d -- uses the Absoft Fortran compiler
make -f makepc surface2ddec -uses the Visual Fortran compiler
make -f makepc waferxy2d - uses the Absoft Fortran compiler
make -f makepc waferxy2ddec-uses the Visual Fortran compiler

9.2 param.h and init2d.h files

Icarus does not use dynamic memory allocation for its arrays since parallel computers typically have defined memory resources per processor; a single program executable can be compiled for any number of processor configurations. The particular problem memory requirements are implemented via two parameter statement blocks: param.h for Icarus and most of the utility programs and init2d.h for the init2d code.

Note: Icarus and the utility programs will check for program limits write and respond with diagnostic messages.

param.h

example mp version of param.h

```
      integer gmre,gcon,ggrd,gmob,gmse,gmss,gpro,gbuf
      integer gmnre,gmrea,gmpcm,gstat,gmwaf,gmtab
      integer gmrx,movie,gmcp,gmcgp,gfield,maxk

        parameter (gmre=10,ggrd=1000,gmse=500)
        parameter (gmob=200,gcon=500)
        parameter (gmss=6)
        parameter (gpro=1024,gbuf=800000)
        parameter (gmrea=23,gmpcm=2,gstat=9)
        parameter (gmwaf=50,gmtab=5,gmrx=20)
        parameter (movie=2,gmcgp=6,gfield=1)
        parameter (icover=0, iplasma=1, ipoisson=1)

      integer lmce,lmmo,lmob

c      parameter (lmce=3510,lmmo=50000,lmob=250)
      parameter (lmce=10000,lmmo=500000,lmob=200,lmcp=1000)

      parameter (eps=1.0E-6,maxk=5)
```

The parameters which start with ‘g’ are global and apply to all processors; those which start with an ‘l’ apply only to a single processor. For a single processor executable, the quantities with the ‘l’ are the total program limits and for a MP executable, the local cell requirements are dictated by the number of processors which are used (see the output from decomp2d). (init2d output contains many of these quantities parameters)

gmre -max. number of grid regions
ggrd -max number of grid lines
gmse -max. number of surface elements
gmob -max. number of outer boundary elements
gcon -max number of region connections
gmss -max. number of chemical species
gpro -max number of mp processors
gbuf -size of global buffer array
gmrea -max. number of chemical and e- impact reactions
gmpcm-max number of reactant pair channels
gstat -dimension of the statistics array for determining moments (use 9 for typical calcs)
gmwaf -max. number of ‘wafer’ surface elements
gmtab -max. number of surface reaction tables
gmrx -max number of surface reactions per table
movie - 2 for non-movie simulations
3 for movie simulations
gmcgp -max number of collision groups (for DSMC binary collisions)
1- for neutral calcs w/o trace species
add 2 for trace species (trace-full and trace-tract collsions)
add 2 for plasmas (ion-neutral and ion-ion collisions)
gfield -number of electro-static fields(2 or 4)
icover - 0 - no coverage model
1 - coverage model data structures
iplasma- 0 - neutral transport only
1 - neutral & ion transport
ipoisson-0 - Poisson equation not performed
1 - Poisson equation data structures
lmce -max. number of local (or single processor) number of cells
lmmo -max. number of local (or single processor) number of particles
lmob -max. number of local (or single processor) number of outer boundaries
lmcp -max. number of local grid corner points
eps -value to check for round-off precison (typically 1.e-6) (meters)
maxk - max. number of loops to determine particle move in a single time step (5)

init2d.h

example init2d.h (parameter section)

```
c
c     include for program init2d   version 6.0
c
     parameter (   m13 = 201,  m24 = 201,    mnc = 500000,
    1            mas = 100,   mie  = 5000,  mntab = 4, mnrx=20,
    2            mmi = 50,    mnvt = 1,     mdsp = 10,
    3            mnre= 2,    mob  = 1300,
    4            mpcm= 2,    mrea = 23,    msd  = m13*2+m24*2,
    5            mse = 5500, msp  = 10,    mtbp = 4,
    6            mnr  = 100,  mac  = 50,
    7            meb = 2*(m13+m24-1)*mnr,  mcpt = mnr * 4,
    8            mcp = 2*mnc,              msce = mse,
    9            mmp = 3,    mccp = 2*mnc, mnb  = 5000,
    a            mng = (m13+m24+2), eps=1.e-6  )

     character*130 title
```

typical values which may require adjustment:

m13 -max. number of grid lines along region side 1 or side 3 (number of cells + 1)
m24 -max. number of grid lines along region side 2 or side 4 (number of cells + 1)
mnc -max. number of computational cells
mrea -max. number of chemical reactions
mse -max. number of surface elements
msp -max. number of chemical species
mnr -max. number of grid regions

9.3 MPI

Icarus, V10, has been written to use the MPI parallel communication protocol. MPI libraries can be obtained on the web for Unix based system. The commercial product, MPI-Pro, from MPI Software Technology, has been successfully used on NT and W2000 single, quad, and cluster configurations by the authors. A simple, single processor emulation set of routines is found in 'single.f' and is used routinely by the authors when using a symbolic debugger. Obtaining MPI libraries are the users' responsibility.

10.0 Miscellaneous Information

10.1 Important Relationships

Conversions:
1 Pascal (N/m^2) = 7.50075 mtorr
1 sccm = $4.48 \cdot 10^{17}$ # molecules/s
1 bar = 10^5 Pa = 0.9869 atm
1 mtorr = 0.133 Pa

Sonic Orifice:

$T^* = (2 / (\gamma+1))\ To$
$V^* = (\gamma R T^*)^{1/2}$

where: T^* = temperature at sonic plane
V^* = velocity at sonic plan
To = stagnation temperature
γ = ratio of specific heats (1.4 for air)
R = ideal gas constant

$R = \mathbf{R}/m$
R = 8.3144 N-m/gmole-K
m = molecular wt

(note: multiply by 1000 for MKS units, kg)

10.2 Chemical Species Database.

*Values from transport chemkin, origin of transport properties not clear
*Values include those from Bird's DSMC Book
*effective diameter calculated at 300 K.
*viscosity coefficient fit from (default @ 273-500 K). -- mu ~ T^s, where s =visc.index
* file created 19 Dec. 1994 -- J. E. Johannes - SNL

*Species	Charge	Atomic wt(Kg)	Molecular wt	Diameter (m)	visc index	Rot. Rel. Coll. #	# Rot.Deg. Freedom	Vib. Rel. Coll. #	Vib. Temp. (K)
AR	0.0	.6633E-25	39.95	.3555E-09	0.8100	5.0	0.0	0.0	0.
AS	0.0	.1244E-24	74.92	.7777E-09	0.8968	5.0	0.0	0.0	0.
AS2	0.0	.2488E-24	149.84	.9356E-09	0.8968	5.0	2.0	0.0	0.
ASH	0.0	.1261E-24	75.93	.4831E-09	0.8734	5.0	0.0	0.0	0.
ASH2	0.0	.1277E-24	76.94	.4945E-09	0.9107	5.0	0.0	0.0	0.
ASH3	0.0	.1294E-24	77.95	.5051E-09	0.9433	5.0	0.0	0.0	0.
C	0.0	.1994E-25	12.01	.3232E-09	0.6902	5.0	0.0	0.0	0.
C2	0.0	.3988E-25	24.02	.3678E-09	0.7246	5.0	2.0	0.0	0.
C2H	0.0	.4156E-25	25.03	.4748E-09	0.8855	5.0	0.0	0.0	0.
C2H2	0.0	.4323E-25	26.04	.4748E-09	0.8856	5.0	0.0	0.0	0.
C2H3	0.0	.4490E-25	27.05	.4748E-09	0.8856	5.0	0.0	0.0	0.
C2H4	0.0	.4658E-25	28.05	.4934E-09	0.9631	5.0	0.0	0.0	0.
C2H5	0.0	.4825E-25	29.06	.5204E-09	0.9349	5.0	0.0	0.0	0.
C2H6	0.0	.4993E-25	30.07	.5204E-09	0.9349	5.0	0.0	0.0	0.
C2N	0.0	.6314E-25	38.03	.4541E-09	0.9138	5.0	0.0	0.0	0.
C2N2	0.0	.8639E-25	52.04	.5733E-09	1.0077	5.0	0.0	0.0	0.
C2O	0.0	.6645E-25	40.02	.4541E-09	0.9137	5.0	0.0	0.0	0.
C3H2	0.0	.6317E-25	38.05	.4748E-09	0.8855	5.0	0.0	0.0	0.
C3H2(S)	0.0	.6317E-25	38.05	.4748E-09	0.8855	5.0	0.0	0.0	0.
C3H4	0.0	.6652E-25	40.07	.5756E-09	0.9346	5.0	0.0	0.0	0.
C3H4P	0.0	.6652E-25	40.07	.5756E-09	0.9346	5.0	0.0	0.0	0.
C3H6	0.0	.6987E-25	42.08	.6111E-09	0.9500	5.0	0.0	0.0	0.
C3H8	0.0	.7321E-25	44.10	.6108E-09	0.9469	5.0	0.0	0.0	0.
C4H	0.0	.8144E-25	49.05	.6858E-09	1.0234	5.0	0.0	0.0	0.
C4H2	0.0	.8312E-25	50.06	.6858E-09	1.0235	5.0	0.0	0.0	0.
C4H6	0.0	.8981E-25	54.09	.6851E-09	1.0118	5.0	0.0	0.0	0.
C4H8	0.0	.9316E-25	56.11	.6852E-09	1.0234	5.0	0.0	0.0	0.
C5H2	0.0	.1031E-24	62.07	.6858E-09	1.0235	5.0	0.0	0.0	0.
C5H5	0.0	.1081E-24	65.10	.6858E-09	1.0235	5.0	0.0	0.0	0.
C6H2	0.0	.1230E-24	74.08	.6858E-09	1.0235	5.0	0.0	0.0	0.
C6H5	0.0	.1280E-24	77.11	.7367E-09	1.0526	5.0	0.0	0.0	0.
C6H5(L)	0.0	.1280E-24	77.11	.7367E-09	1.0526	5.0	0.0	0.0	0.
C6H5O	0.0	.1546E-24	93.11	.7760E-09	1.0658	5.0	0.0	0.0	0.
C6H6	0.0	.1297E-24	78.11	.7367E-09	1.0526	5.0	0.0	0.0	0.
C6H7	0.0	.1314E-24	79.12	.7367E-09	1.0525	5.0	0.0	0.0	0.
CH	0.0	.2162E-25	13.02	.2726E-09	0.6933	5.0	2.0	0.0	0.
CH2	0.0	.2329E-25	14.03	.4087E-09	0.7845	5.0	0.0	0.0	0.
CH2(S)	0.0	.2329E-25	14.03	.4087E-09	0.7845	5.0	0.0	0.	0.0
CH2CHCCH	0.0	.8646E-25	52.08	.6858E-09	1.0235	5.0	0.0	0.0	0.
CH2CHCCH2	0.0	.8814E-25	53.08	.6858E-09	1.0235	5.0	0.0	0.0	0.

CH2CHCH2	0.0	.6819E-25	41.07	.5907E-09	0.9392	5.0	0.0	0.0	0.
CH2CHCHCH	0.0	.8814E-25	53.08	.6858E-09	1.0235	5.0	0.0	0.0	0.
CH2(CH)2CH2	0.0	.8981E-25	54.09	.6858E-09	1.0235	5.0	0.0	0.0	0.
CH2CO	0.0	.6980E-25	42.04	.5553E-09	1.0614	5.0	0.0	0.0	0.
CH2O	0.0	.4985E-25	30.03	.5206E-09	1.0747	5.0	0.0	0.0	0.
CH2OH	0.0	.5153E-25	31.03	.5164E-09	1.0386	5.0	0.0	0.0	0.
CH3	0.0	.2496E-25	15.04	.4093E-09	0.7969	5.0	0.0	0.0	0.
CH3CC	0.0	.6485E-25	39.06	.5756E-09	0.9345	5.0	0.0	0.0	0.
CH3CCCH2	0.0	.8814E-25	53.08	.6851E-09	1.0118	5.0	0.0	0.0	0.
CH3CCCH3	0.0	.8981E-25	54.09	.6851E-09	1.0118	5.0	0.0	0.0	0.
CH3CCH2	0.0	.6819E-25	41.07	.5911E-09	0.9435	5.0	0.0	0.0	0.
CH3CH2CCH	0.0	.8981E-25	54.09	.6851E-09	1.0118	5.0	0.0	0.0	0.
CH3CHCH	0.0	.6819E-25	41.07	.5911E-09	0.9435	5.0	0.0	0.0	0.
CH3CO	0.0	.7147E-25	43.05	.5539E-09	1.0353	5.0	0.0	0.0	0.
CH3O	0.0	.5153E-25	31.03	.5150E-09	1.0120	5.0	0.0	0.0	0.
CH3OH	0.0	.5320E-25	32.04	.5194E-09	1.0386	5.0	0.0	0.0	0.
CH4	0.0	.2664E-25	16.04	.4022E-09	0.8400	5.0	0.0	0.0	0.
CL	0.0	.5886E-25	35.45	.3831E-09	0.7762	5.0	0.0	0.0	0.
CL+	1.0	.5886E-25	35.45	.3831E-09	0.7762	5.0	0.0	0.0	0.
CL-	-1.0	.5886E-25	35.45	.3831E-09	0.7762	5.0	0.0	0.0	0.
CL2+	1.0	.1177E-25	70.91	.5405E-09	1.0100	5.0	2.0	0.0	0.
CL2	0.0	.1177E-24	70.91	.5405E-09	1.0100	5.0	2.0	0.0	0.
CN	0.0	.4320E-25	26.02	.3798E-09	0.6942	5.0	2.0	0.0	0.
CNN	0.0	.6645E-25	40.02	.4541E-09	0.9138	5.0	0.0	0.0	0.
CO	0.0	.4651E-25	28.01	.3710E-09	0.7254	5.0	2.0	0.0	0.
CO2	0.0	.7307E-25	44.01	.4516E-09	0.9264	5.0	0.0	0.0	0.
e	-1	.9049E-30	0.00	.6941E-07	0.9523	5.0	0.0	0.0	0.
F	0.0	.3154E-25	19.00	.2728E-09	0.7005	5.0	0.0	0.0	0.
F2	0.0	.6309E-25	38.00	.3477E-09	0.7680	5.0	2.0	0.0	0.
GA	0.0	.1158E-24	69.72	.9372E-09	0.8264	5.0	0.0	0.0	0.
GAH	0.0	.1174E-24	70.73	.5515E-09	1.0002	5.0	2.0	0.0	0.
GAME	0.0	.1407E-24	84.76	.8246E-09	0.9151	5.0	0.0	0.0	0.
GAME2	0.0	.1657E-24	99.79	.8123E-09	1.0043	5.0	0.0	0.0	0.
GAME3	0.0	.1906E-24	114.83	.7414E-09	1.0208	5.0	0.0	0.0	0.
H	0.0	.1674E-26	1.01	.2211E-09	0.7984	5.0	0.0	0.0	0.
H2	0.0	.3347E-26	2.02	.2701E-09	0.6700	5.0	2.0	0.0	0.
H2C4O	0.0	.1097E-24	66.06	.6851E-09	1.0118	5.0	0.0	0.0	0.
H2CCC	0.0	.6317E-25	38.05	.4748E-09	0.8855	5.0	0.0	0.0	0.
H2CCC(S)	0.0	.6317E-25	38.05	.4748E-09	0.8855	5.0	0.0	0.0	0.
H2CCCCH	0.0	.1047E-24	63.08	.6851E-09	1.0118	5.0	0.0	0.0	0.
H2CCCCH	0.0	.8479E-25	51.07	.6851E-09	1.0118	5.0	0.0	0.0	0.
H2CCCCH2	0.0	.8646E-25	52.08	.6851E-09	1.0119	5.0	0.0	0.0	0.
H2CCCH	0.0	.6485E-25	39.06	.5756E-09	0.9345	5.0	0.0	0.0	0.
H2CN	0.0	.4654E-25	28.03	.5424E-09	1.0303	5.0	0.0	0.0	0.
H2NO	0.0	.5317E-25	32.02	.3636E-09	0.7535	5.0	0.0	0.0	0.
H2O	0.0	.2991E-25	18.02	.4387E-09	1.0855	5.0	0.0	0.0	0.
H2O2	0.0	.5647E-25	34.01	.3555E-09	0.7310	5.0	0.0	0.0	0.
H2S	0.0	.5658E-25	34.08	.4551E-09	0.9799	5.0	0.0	0.0	0.
H2SISIH2	0.0	.9996E-25	60.20	.5875E-09	0.9862	5.0	0.0	0.0	0.
H3SISIH	0.0	.9996E-25	60.20	.5875E-09	0.9862	5.0	0.0	0.0	0.
HCCCHCCH	0.0	.1047E-24	63.08	.6858E-09	1.0235	5.0	0.0	0.0	0.

HCCHCC	0.0	.8479E-25	51.07	.6858E-09	1.0235	5.0	0.0	0.0	0.
HCCO	0.0	.6812E-25	41.03	.2707E-09	0.7924	5.0	0.0	0.0	0.
HCCOH	0.0	.6980E-25	42.04	.5553E-09	1.0614	5.0	0.0	0.0	0.
HCL	0.0	.6054E-25	36.46	.4396E-09	0.9953	5.0	2.0	0.0	0.
HCN	0.0	.4487E-25	27.03	.5452E-09	1.0774	5.0	0.0	0.0	0.
HCNO	0.0	.7143E-25	43.03	.4537E-09	0.9067	5.0	0.0	0.0	0.
HCO	0.0	.4818E-25	29.02	.5206E-09	1.0747	5.0	0.0	0.0	0.
HCO+	1.0	.4818E-25	29.02	.5206E-09	1.0748	5.0	0.0	0.0	0.
HE	0.0	.6646E-26	4.00	.2157E-09	0.6330	5.0	0.0	0.0	0.
HF	0.0	.3322E-25	20.01	.4598E-09	1.0871	5.0	2.0	0.0	0.
HNCO	0.0	.7143E-25	43.03	.4537E-09	0.9067	5.0	0.0	0.0	0.
HNNO	0.0	.7475E-25	45.02	.4537E-09	0.9067	5.0	0.0	0.0	0.
HNO	0.0	.5149E-25	31.01	.3632E-09	0.7437	5.0	0.0	0.0	0.
HNOH	0.0	.5317E-25	32.02	.3632E-09	0.7437	5.0	0.0	0.0	0.
HO2	0.0	.5480E-25	33.01	.3555E-09	0.7311	5.0	0.0	0.0	0.
HOCN	0.0	.7143E-25	43.03	.4537E-09	0.9067	5.0	0.0	0.0	0.
He	0.0	.3340E-26	4.02	.2333E-09	0.6600	5.0	0.0	0.0	0.
I*C3H7	0.0	.7154E-25	43.09	.6111E-09	0.9500	5.0	0.0	0.0	0.
K	0.0	.6492E-25	39.10	.6944E-09	0.9523	5.0	0.0	0.0	0.
K+	1.0	.6492E-25	39.10	.6944E-09	0.9523	5.0	0.0	0.0	0.
KCL	0.0	.1238E-24	74.56	.7964E-09	0.8441	5.0	2.0	0.0	0.
KH	0.0	.6659E-25	40.11	.3578E-09	0.7186	5.0	2.0	0.0	0.
KO	0.0	.9148E-25	55.10	.5137E-09	1.0227	5.0	2.0	0.0	0.
KOH	0.0	.9316E-25	56.11	.7879E-09	0.8647	5.0	2.0	0.0	0.
Kr	0.0	.1391E-24	83.80	.4760E-09	0.8000	5.0	0.0	0.0	0.
N	0.0	.2326E-25	14.01	.3229E-09	0.6825	5.0	0.0	0.0	0.
N*C3H7	0.0	.7154E-25	43.09	.6108E-09	0.9469	5.0	0.0	0.0	0.
N2	0.0	.4651E-25	28.01	.3675E-09	0.7400	5.0	2.0	0.0	0.
N2H2	0.0	.4986E-25	30.03	.3718E-09	0.6825	5.0	0.0	0.0	0.
N2H3	0.0	.5153E-25	31.04	.4469E-09	0.8645	5.0	0.0	0.0	0.
N2H4	0.0	.5320E-25	32.05	.4872E-09	0.8711	5.0	0.0	0.0	0.
N2O	0.0	.7307E-25	44.01	.4537E-09	0.9067	5.0	0.0	0.0	0.
NCN	0.0	.6645E-25	40.02	.4541E-09	0.9139	5.0	0.0	0.0	0.
NCO	0.0	.6976E-25	42.02	.4541E-09	0.9139	5.0	0.0	0.0	0.
NH	0.0	.2493E-25	15.01	.2628E-09	0.6989	5.0	2.0	0.0	0.
NH2	0.0	.2660E-25	16.02	.2628E-09	0.6988	5.0	0.0	0.0	0.
NH3	0.0	.2828E-25	17.03	.4290E-09	1.1000	5.0	0.0	0.0	0.
NNH	0.0	.4818E-25	29.02	.3721E-09	0.6886	5.0	0.0	0.0	0.
NO	0.0	.4982E-25	30.01	.3678E-09	0.7900	5.0	2.0	0.0	0.
NO2	0.0	.7638E-25	46.01	.4014E-09	0.8733	5.0	0.0	0.0	0.
Ne	0.0	.3350E-25	20.80	.2770E-09	0.6600	5.0	0.0	0.0	0.
O	0.0	.2656E-25	16.00	.2727E-09	0.6989	5.0	0.0	0.0	0.
O2	0.0	.5313E-25	32.00	.3558E-09	0.7700	5.0	2.0	0.0	0.
O3	0.0	.7969E-25	48.00	.4601E-09	0.8455	5.0	0.0	0.0	0.
OH	0.0	.2824E-25	17.01	.2727E-09	0.6988	5.0	2.0	0.0	0.
S	0.0	.5324E-25	32.06	.6273E-09	0.9600	5.0	0.0	0.0	0.
S2	0.0	.1065E-24	64.13	.6373E-09	0.9600	5.0	2.0	0.0	0.
SH	0.0	.5491E-25	33.07	.6373E-09	0.9600	5.0	2.0	0.0	0.
SI	0.0	.4663E-25	28.09	.5923E-09	0.8241	5.0	2.0	0.0	0.
SI2	0.0	.9326E-25	56.17	.6676E-09	0.8241	5.0	2.0	0.0	0.
SI2H2	0.0	.9661E-25	58.19	.5651E-09	0.9974	5.0	0.0	0.0	0.

SI2H3	0.0	.9828E-25	59.20	.5768E-09	0.9937	5.0	0.0	0.0	0.
SI2H5	0.0	.1016E-24	61.21	.5997E-09	0.9856	5.0	0.0	0.0	0.
SI2H6	0.0	.1033E-24	62.22	.6109E-09	0.9814	5.0	0.0	0.0	0.
SI3	0.0	.1399E-24	84.26	.7225E-09	0.8241	5.0	0.0	0.0	0.
SI3H8	0.0	.1533E-24	92.32	.7210E-09	0.9975	5.0	0.0	0.0	0.
SICL2	0.0	.1647E-24	98.00	.8000E-09	0.8386	5.0	2.0	0.0	0.
SICL4	0.0	.2821E-24	169.90	.5428E-09	0.8363	5.0	0.0	0.0	0.
SIF3	0.0	.1413E-24	85.08	.5554E-09	0.9876	5.0	0.0	0.0	0.
SIF3NH2	0.0	.1679E-24	101.10	.5894E-09	0.9122	5.0	0.0	0.0	0.
SIF4	0.0	.1728E-24	104.08	.5428E-09	0.8363	5.0	0.0	0.0	0.
SIH	0.0	.4830E-25	29.09	.3711E-09	0.7206	5.0	0.0	0.0	0.
SIH2	0.0	.4998E-25	30.10	.4041E-09	0.7776	5.0	0.0	0.0	0.
SIH3	0.0	.5165E-25	31.11	.4377E-09	0.8320	5.0	0.0	0.0	0.
SIH4	0.0	.5333E-25	32.12	.4722E-09	0.8826	5.0	0.0	0.0	0.
SIHF3	0.0	.1429E-24	86.09	.5258E-09	0.8485	5.0	0.0	0.0	0.
SO	0.0	.7980E-25	48.06	.5051E-09	0.9811	5.0	2.0	0.0	0.
SO2	0.0	.1064E-24	64.06	.5188E-09	1.0500	5.0	0.0	0.0	0.
SO3	0.0	.1329E-24	80.06	.5611E-09	1.0261	5.0	0.0	0.0	0.
Xe	0.0	.2180E-24	131.29	.5740E-09	0.8500	5.0	0.0	0.0	0.0

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12.0 Papers

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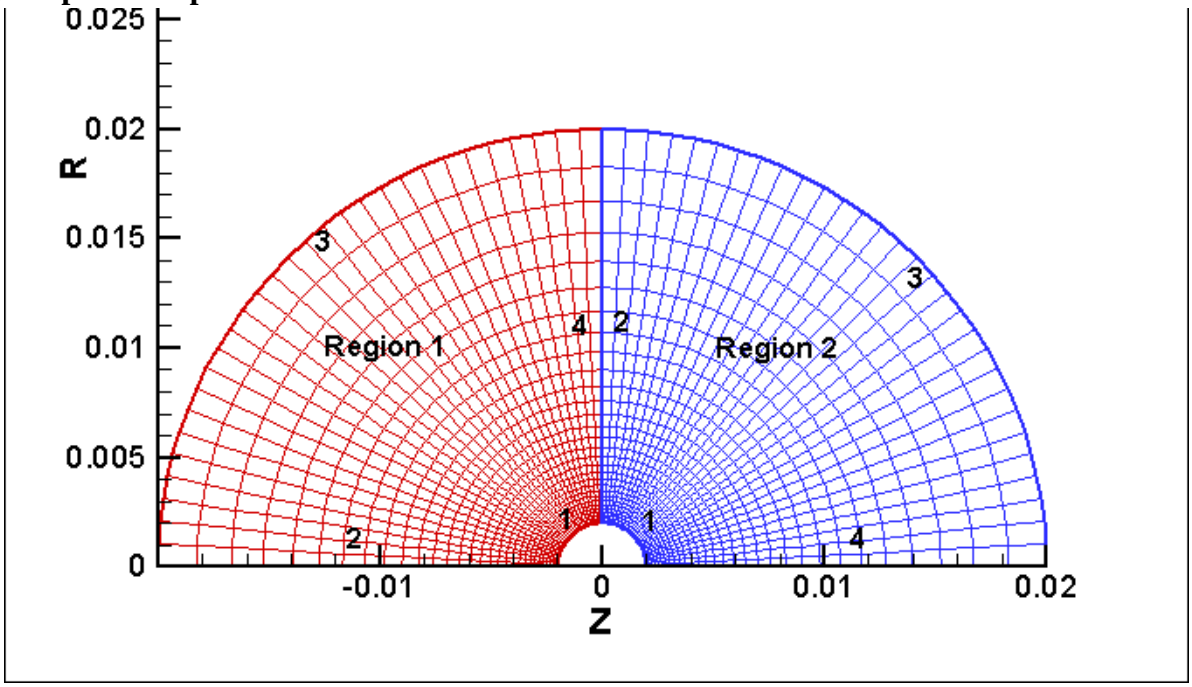
13.0 Sample Problems

13.1 ICF Sphere

Purpose: Simulate the heat transfer for an ICF sphere injected into the chamber. This illustrated the strategy to grid a curved surface. The sphere is simply an axisymmetric version of the cross-flow cylinder situation. Note that a single region cannot be used since the method to determine particle location does not work when side 2 is *below* side 4 for a portion of the domain and *above* for another portion. The first file, sphere2.inp, shows a simple 2 region configuration. The second file, spherez.inp illustrates a generic problem with axisymmetric particle methods: radial weight factors effect the stagnation point. To minimize this problem, adding a grid which is basically uniform along the centerline will cause the cell weights to be axially similar; this minimizes the effect of cloning.

grid sphere2.inp



fille sphere2.inp (2 region)

```
*-------------------------------------------------------------------
*   asterick in column 1 indicates comment card
*-------------------------------------------------------------------
*
 ICF target sphere
*
*
*-------------------------------------------------------------------
*
control    1      -1 -- plot grid only;
*                  1 -- initialization & plot file
*
type       1              0/1 for X-Y or Z-R flow
*
read general grid
```

```
*---------------------------------------------------------------------
*                  Region Definition
*---------------------------------------------------------------------
    2          number of regions (must be .le. 30)
    6          number of global points (must be .le.120)
*--------------------------------------
*    Global corner pt. coordinates
*  Pt.       z (m)          r(m)
*--------------------------------------
1  -0.02    0.
2  -0.002    0.0
3   0.002    0.0
4   0.02   0.0
5   0.0    0.002
6   0.0    0.02
*---------------------------------------------------------------------
*           Individual Region Definitions Follow
*           --REGION NUMBERS MUST BE SEQUENTIAL--
*---------------------------------------------------------------------
*=====================================================================
region   1  <------  Inputs specific to this region follow
*=====================================================================
grid
   2            global points
   1
   6
   5
   30          number of cells along sides 1 and 3
   30            number of cells along sides 2 and 4
   1             sides 1 and 3 curvature: 0/1 for line/circular arc
   0             sides 1 and 3 cell spacing:
   2  1.1   150.           sides 2 and 4 cell spacing:
   5             boundary type code for sides 1 - 4, resp.
   1
   3
   7
   3
*---------------------------------------------------------------------
*   Side  Cell1  Cell2   elem/cell  Spec. refl.   Temp. K    Material#    Value
*---------------------------------------------------------------------
    1     1     5       1            0.000       18.00        0          0.
    1     6     15      3            0.000       18.00        0          0.
    1     16    500     1            0.000       18.00        0          0.
*---------------------------------------------------------------------
*                 Region interface/matching
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*---------------------------------------------------------------------
       1          0
       2          0
       3          0
       4          1           2    2
```

```
*========================================================================
*========================================================================
region   2  <------  Inputs specific to this region follow
*========================================================================
grid
   5            global points
   6
   4
   3
   30          number of cells along sides 1 and 3
   30            number of cells along sides 2 and 4
   1             sides 1 and 3 curvature: 0/1 for line/circular arc
   0             sides 1 and 3 cell spacing:
   2  1.1   150.            sides 2 and 4 cell spacing:
   5             boundary type code for sides 1 - 4, resp.
   7
   3
   1
   1
*------------------------------------------------------------------------
*   Side  Cell1  Cell2   elem/cell  Spec. refl.   Temp. K    Material#    Value
*------------------------------------------------------------------------
    1     1     500       1          0.000       18.00        0           0.
*------------------------------------------------------------------------
*                  Region interface/matching
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*------------------------------------------------------------------------
       1          0
       2          1        4    1
       3          0
       4          0
*========================================================================
*========================================================================
*------------------------------------------------------------------------
END                 END OF EXPERT INPUT FILE
*------------------------------------------------------------------------
```

file: inlet (specify freestream conditions)

```
*
*   freestream inlet condition for the ICF sphere
*
*      Xe species
*
1 number of tables
*
0   -----  flag to specify freestream conditions
3.216e20   400.    0.0     1500.   1500.   1500.    1.
*
```

file: spec (only translational modes simulated, extra input in file)

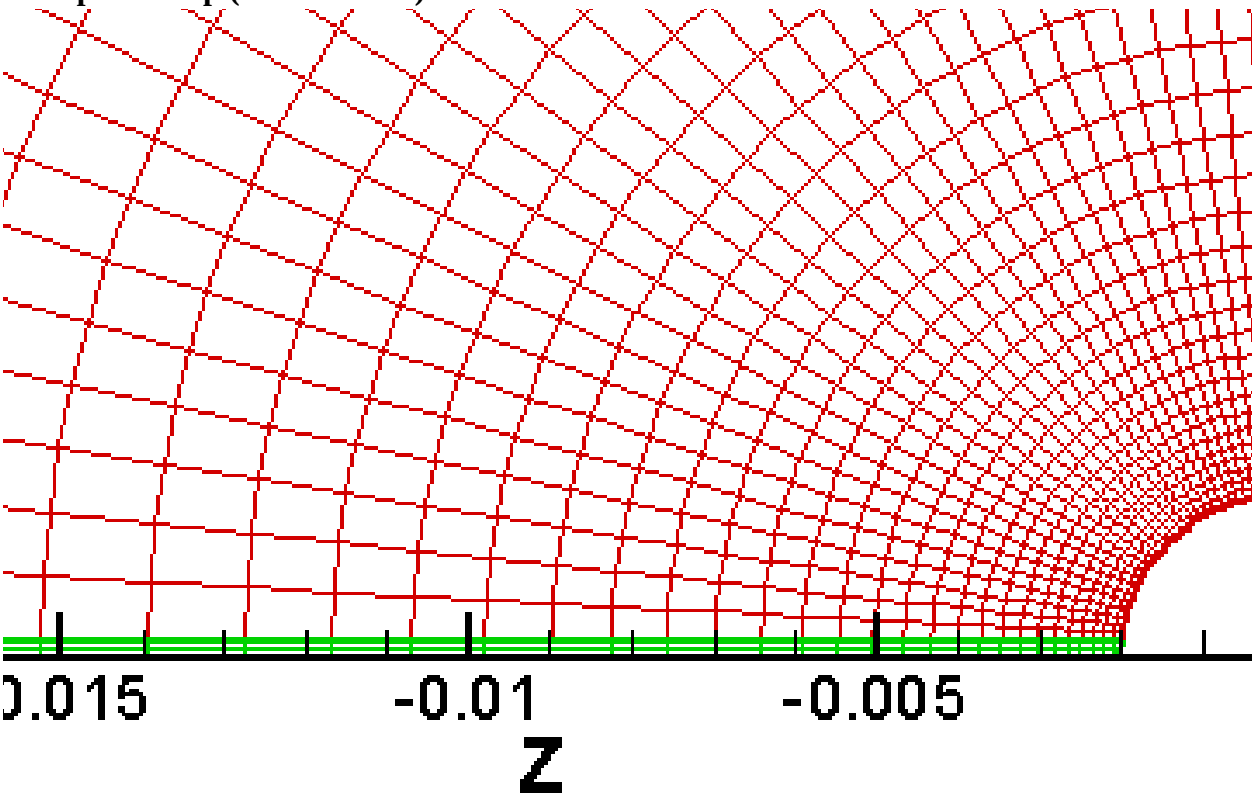
```
****************************************
*      species data file           *
****************************************
1          number of species
*
3          internal structure of most complex molecule:
*          3-monatomic, 4-rotation, 5-rotat. + vibrat.
*
0          # of chemical reactions
*
*-------------------------------------------------------------------------------------------------------------------
* ID
* Mwt    Mol. mass   Diam.   #Rot.Deg.    Rot.Rel.  # Vib. Deg.  Vib. Rel. Vib.Temp. specie wt. charge   omega   tref   alpha
*          (kg)       (m)     Freedom      Coll. #    Freedom      Coll. #     (K)
*-------------------------------------------------------------------------------------------------------------------
 Xe
 131.229  2.18e-25  5.74e-10      0.         5.         0.          0.         0.       1.0      0.0      .85    300.     1.
*
END

 O2
 32.00    5.31E-26  3.96E-10      2.       5.       50.       2270.          1.0      0.0
 N2
 28.016   4.65E-26  4.07E-10      2.       5.       50.       3390.          1.0      0.0
 O
 16.00    2.65E-26    3.E-10      0.       0.        0.         0.           1.0      0.0
 N
 14.008  2.325E-26    3.E-10      0.       0.        0.         0.           1.0      0.0
 NO
 30.008   4.98E-26    4.E-10      2.       5.       50.       2740.          1.0      0.0
```

screen output from init2d:

```
 init2d for Icarus -- version 10.00f


opening input file sphere2.inp


opening species file spec
finished with file spec

opening inlet file inlet
finished reading file inlet

starting region   1
starting region   2
```

```
total cell volume(m^3) =   3.345388E-05

values in () pertain to param.h limits

initial molecules based on   20  min per cell

  34436  molecules in initial grid
  2  regions (gmre)
  1800  computational cells (gmce)
  1  chemical species (gmss)


  14  region connections (gcon)
  124  grid data size (ggrd)
  60  boundary elements (gmob)
  80  surface elements (gmse)
  1922  cell corner points (gmcp)
  60  inlet table boundary cells
  0  pumps or pressure points
  0  # of wafer elements (gmwaf)


 species definition file =          spec
 inlet flow boundary file =         inlet
 output grid file =                 grid
 output problem definition file =   datap
 summary output file =              init2dout
```

file: spherez.inp (zoomed view)



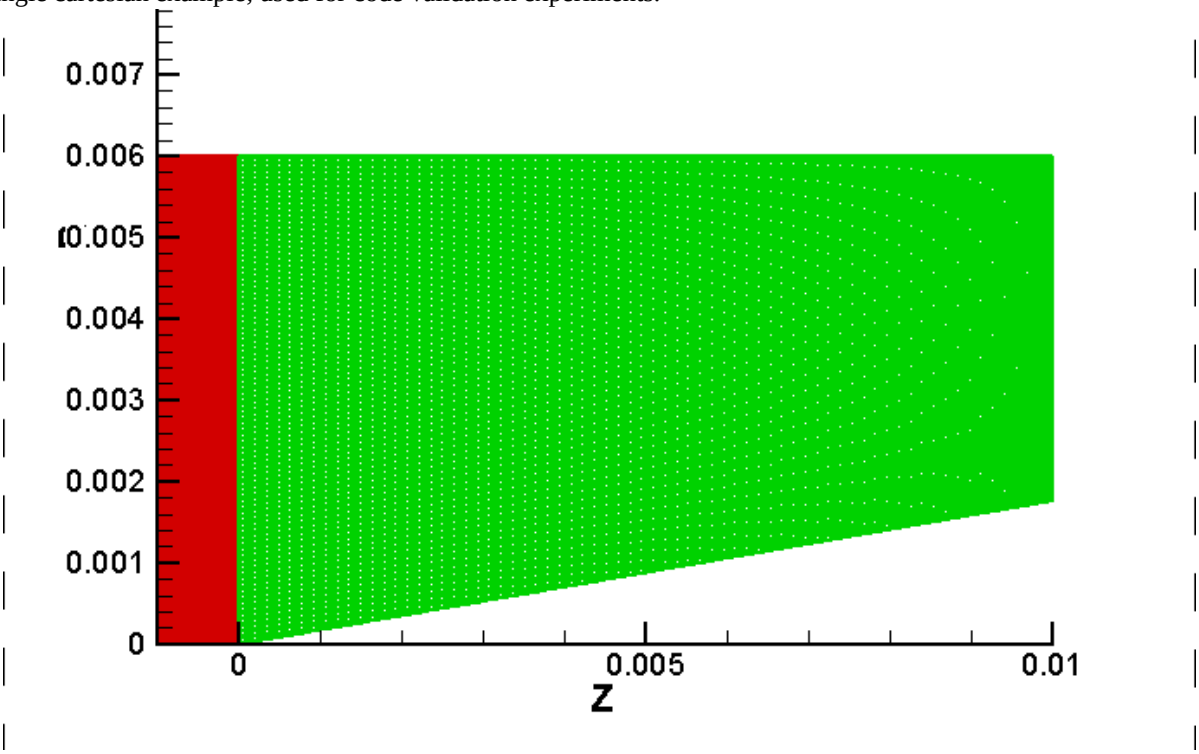

```
*---------------------------------------------------------------------
*   asterick in column 1 indicates comment card
*---------------------------------------------------------------------
*
 1/2 sphere
*
*
*---------------------------------------------------------------------
*
control    1      -1 -- plot grid only;
*                  1 -- initialization & plot file
*
type       1              0/1 for X-Y or Z-R flow
*
read general grid
*---------------------------------------------------------------------
*                    Region Definition
*---------------------------------------------------------------------
    2          number of regions (must be .le. 30)
    8          number of global points (must be .le.120)
*---------------------------------------
```

```
*     Global corner pt. coordinates
*  Pt.        z (m)          r(m)
*-------------------------------------
1  -0.02    0.
2  -0.002    0.0
3   0.002    0.0
4   0.02   0.0
5   0.0    0.002
6   0.0    0.02
7   -0.0199908     0.000210957
8   -0.00198962    0.00020913
*---------------------------------------------------------------------
*            Individual Region Definitions Follow
*            --REGION NUMBERS MUST BE SEQUENTIAL--
*---------------------------------------------------------------------
*=====================================================================
region   1  <------  Inputs specific to this region follow
*=====================================================================
grid
   8            global points
   7
   6
   5
   30          number of cells along sides 1 and 3
   30            number of cells along sides 2 and 4
   1             sides 1 and 3 curvature: 0/1 for line/circular arc
   0             sides 1 and 3 cell spacing:
   2  1.1   150.            sides 2 and 4 cell spacing:
   5             boundary type code for sides 1 - 4, resp.
   7
   3
   3
   1
*---------------------------------------------------------------------
*   Side  Cell1  Cell2  elem/cell   Spec. refl.   Temp. K    Material#    Value
*---------------------------------------------------------------------
    1     1     500       1          0.000       18.00        0          0.
*---------------------------------------------------------------------
*                 Region interface/matching
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*---------------------------------------------------------------------
       1          0
       2          1    4   2
       3          0
       4          0
*=====================================================================
*=====================================================================
region   2  <------  Inputs specific to this region follow
*=====================================================================
grid
   2            global points
```

```
   1
   7
   8
   2          number of cells along sides 1 and 3
   30            number of cells along sides 2 and 4
   -5   0.002   1    1              sides 1 and 3 curvature: 0/1 for line/circular arc
   0             sides 1 and 3 cell spacing:
   2  1.1   150.            sides 2 and 4 cell spacing:
   5             boundary type code for sides 1 - 4, resp.
   1
   3
   7
   1
*-------------------------------------------------------------------------
*   Side  Cell1  Cell2   elem/cell   Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
    1     1     500         1          0.000       18.00        0          0.
*-------------------------------------------------------------------------
*                 Region interface/matching
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*-------------------------------------------------------------------------
       1          0
       2          0
       3          0
       4          1     2     1
*=========================================================================
*=========================================================================
*-------------------------------------------------------------------------
END               END OF EXPERT INPUT FILE
*-------------------------------------------------------------------------
```

13.2 Wedge

Single cartesian example; used for code validation experiments.



file: wedge.inp

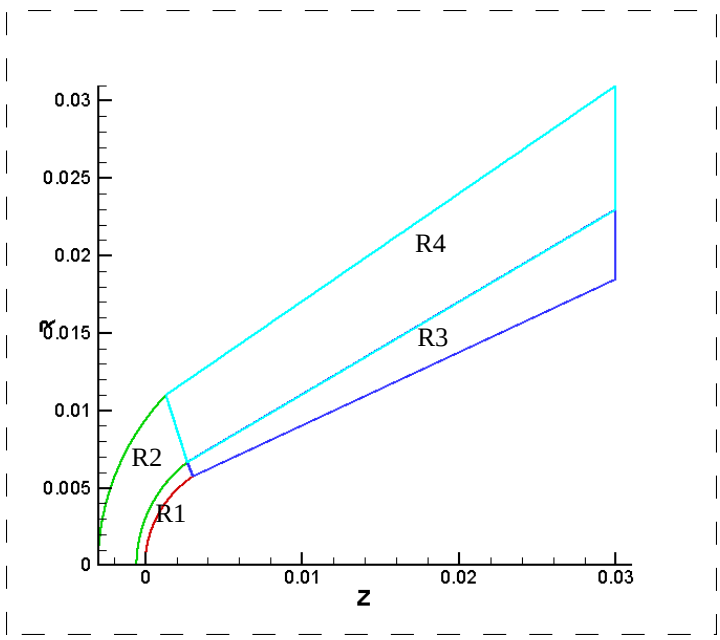
```
*-----------------------------------------------------------------------
*   asterick in column 1 indicates comment card
*-----------------------------------------------------------------------
*
 10 Deg Wedge (FINE)
*
*
*-----------------------------------------------------------------------
*       options section
*-----------------------------------------------------------------------
*
control    1          -1 -- plot grid only;
*                      1 -- initialization & plot file
*
type            0       0/1 for X-Y or Z-R flow
*
cell weight    0
*-----------------------------------------------------------------------
read general grid
*
    2           number of regions
    6           number of global points
*-------------------------------------
*     Global corner pt. coordinates
```

```
*  Pt.       z (m)          r(m)
*---------------------------------------
1  -0.001    0.
2  -0.001  0.006
3   0.     0.006
4   0.   0.0
5   0.01  0.006
6   0.01  0.001763269
*-------------------------------------------------------------------------
*            Individual Region Definitions Follow
*            --REGION NUMBERS MUST BE SEQUENTIAL--
*-------------------------------------------------------------------------
*=========================================================================
region   1  <------  Inputs specific to this region follow
*=========================================================================
grid
   1            global points
   2
   3
   4
   50          number of cells along sides 1 and 3
   200           number of cells along sides 2 and 4
   0             sides 1 and 3 curvature: 0/1 for line/circular arc
   0             sides 1 and 3 cell spacing:
   0             sides 2 and 4 cell spacing:
   5             boundary type code for sides 1 - 4, resp.
   3
   5
   7
   2
*-------------------------------------------------------------------------
*   Side  Cell1  Cell2  #elem/cell   Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
    1    1    500      1         1.000       180.00       0          0.
    3    1    500      1         1.000       180.00       0          0.
*-------------------------------------------------------------------------
*                 Region interface/matching
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*-------------------------------------------------------------------------
        1          0
        2          0
        3          0
        4          1      2       2
*=========================================================================
*=========================================================================
region   2  <------  Inputs specific to this region follow
*=========================================================================
grid
   4            global points
   3
   5
```

```
   6
   400          number of cells along sides 1 and 3
   200           number of cells along sides 2 and 4
   0            sides 1 and 3 curvature: 0/1 for line/circular arc
   0            sides 1 and 3 cell spacing:
   0            sides 2 and 4 cell spacing:
   5            boundary type code for sides 1 - 4, resp.
   7
   5
   3
   2
*-------------------------------------------------------------------------
*  Side  Cell1  Cell2  #elem/cell    Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
   1    1    500      1          1.000      180.00      0          0.
   3    1    500      1          1.000      180.00      0          0.
*-------------------------------------------------------------------------
*                Region interface/matching
*   Reg. side   reg. sides      Adj. side| Adj. reg.
*-------------------------------------------------------------------------
      1         0
      2         1     4      1
      3         0
      4         0
*=========================================================================
*-------------------------------------------------------------------------
END               END OF EXPERT INPUT FILE
*-------------------------------------------------------------------------
```

13.3 AIAA V&V Spherically Blunted Bi-Conic (reference 12.9)

This problem illustrates the use of multiple regions to cluster cells near areas of interest. The figure shows the grid for the blunted fore-cone of the body; multiple regions are used to currectly capture the bow shock as well as the large increase in density at the surface. The input option for init2d to allow one to use a solution file (either from Icarus or a continuum code in Tecplot format) to 'test' a candidate grid by determining the local cell Kn and time step was very useful in determining the validity of this grid. The figure shows two regions in the direction normal to the surface of the body.




```
------------------------------------------------------------------------
*   asterick in column 1 indicates comment card
*-----------------------------------------------------------------------
*
 AIAA Run 31 - v3c v10 grid
*
*
*-----------------------------------------------------------------------
*
control    1         -1 -- plot grid only;
*                     1 -- initialization & plot file
*
type           1      0/1 for X-Y or Z-R flow
*
cell weight    3
*-----------------------------------------------------------------------
*                   Region Definition
*-----------------------------------------------------------------------
read general grid
*
    4        number of regions (must be .le. 30)
    19           number of global points (must be .le.120)
*-------------------------------------
```

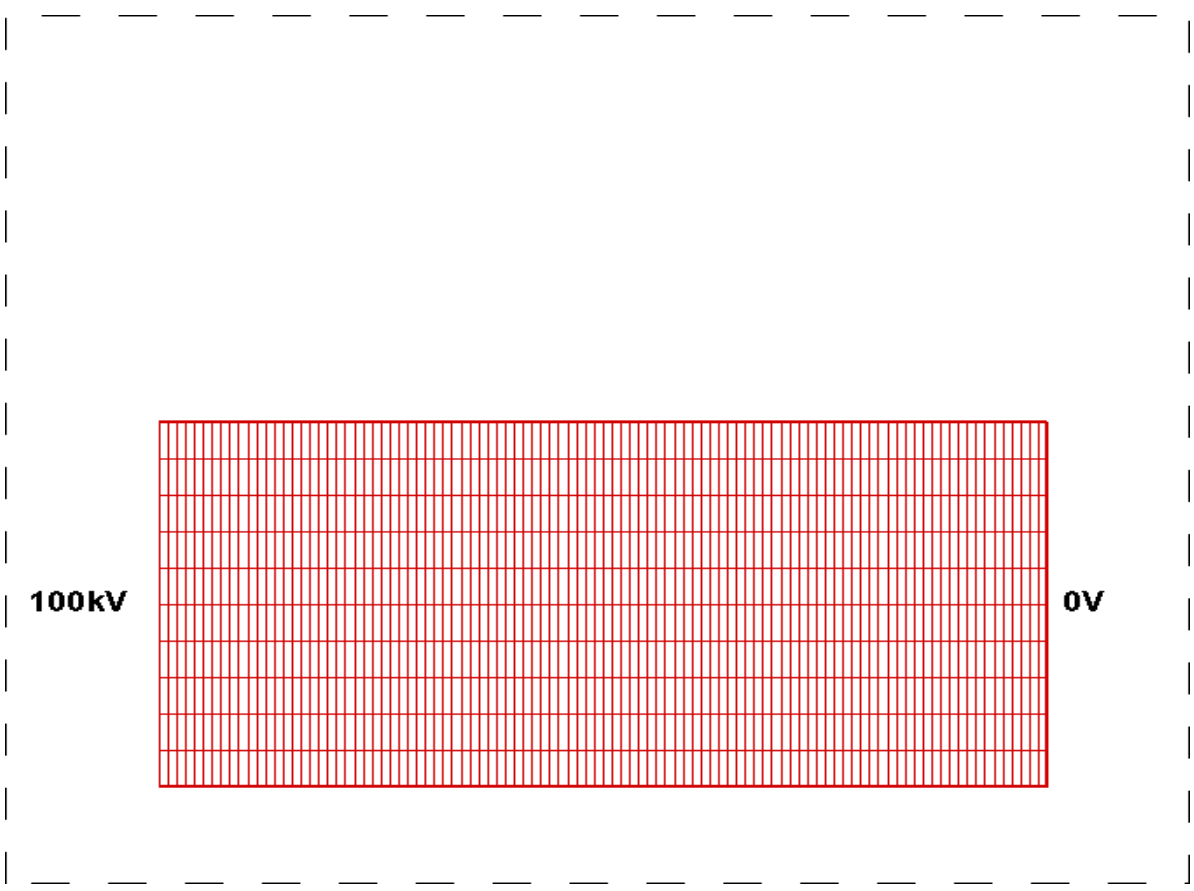
```
*     Global corner pt. coordinates
*  Pt.        z (m)          r(m)
*-------------------------------------
1  -0.003000    0.
2   0.082767    0.0429514
3   0.1443824   0.130937
4   0.184362    0.130937
5  -0.009313    0.01
6   0.030.031
7   0.122957    0.17802          7   0.144695 0.22
8   0.184362    0.22
9  -0.014313    0.0
10 -0.014313    0.008
11  0.000       0.0
12  0.003037    0.005756
13  0.001318    0.011014
14  0.03        0.0185
15  0.03        0.0310.08332
16  0.099472    0.066805       0.11007     0.08149
17  -0.00055    0.000000
18  0.002685    0.00667
19  0.030.023
*---------------------------------------------------------------------
*            Individual Region Definitions Follow
*            --REGION NUMBERS MUST BE SEQUENTIAL--
*---------------------------------------------------------------------
*=====================================================================
region   1  <------  Inputs specific to this region follow
*=====================================================================
grid
   11             global points
   17
   18
   12
   2000           number of cells along sides 1 and 3
   200            number of cells along sides 2 and 4
   1              sides 1 and 3 curvature: 0/1 for line/circular arc
   0            sides 1 and 3 cell spacing
   2  1.02   100.  sides 2 and 4 cell spacing
   5              boundary type code for sides 1 - 4, resp.
   1
   7
   7
   1
*---------------------------------------------------------------------
*   Side  Cell1  Cell2  #elem/cell   Spec. refl.   Temp. K    Material#    Value
*---------------------------------------------------------------------
     1     1    2000      1          .000       297.22        0          0.
*    3     1     500      1          1.000       180.00        0          0.
*---------------------------------------------------------------------
*                 Region interface/matching
```

```
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*-------------------------------------------------------------------------
       1          0
       2          0
       3          1   1    2
       4     1   2    3
*=========================================================================
region   2  <------  Inputs specific to this region follow
*=========================================================================
grid
   17             global points
   1
   13
   18
   1000            number of cells along sides 1 and 3
   250             number of cells along sides 2 and 4
   1              sides 1 and 3 curvature: 0/1 for line/circular arc
   0
   0    2  1.03   1000
   7              boundary type code for sides 1 - 4, resp.
   1
   3
   7
   0
*-------------------------------------------------------------------------
*   Side  Cell1  Cell2   #elem/cell  Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
*     1     1    1000     1         .000       297.22       0          0.
*     3     1     500     1        1.000       180.00       0          0.
*-------------------------------------------------------------------------
*                 Region interface/matching
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*-------------------------------------------------------------------------
       1          1    3    1
       2          0
       3          0
       4     1    2    4
*=========================================================================
region   3  <------  Inputs specific to this region follow
*=========================================================================
grid
   12             global points
   18
   19
   14
   2000            number of cells along sides 1 and 3
   200             number of cells along sides 2 and 4
   0              sides 1 and 3 curvature: 0/1 for line/circular arc
   0              sides 1 and 3 cell spacing:
   0             sides 2 and 4 cell spacing:
   5              boundary type code for sides 1 - 4, resp.
```

```
   7
   7
   3
   1
*-------------------------------------------------------------------------
*   Side  Cell1  Cell2   #elem/cell  Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
    1    1    2000       1          .000       297.22       0          0.
*    3    1     500       1          1.000       180.00       0          0.
*-------------------------------------------------------------------------
*                Region interface/matching
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*-------------------------------------------------------------------------
       1         0
       2         1     4      1
       3         1    1       4
       4         0
*=========================================================================
*=========================================================================
region   4 <------  Inputs specific to this region follow
*=========================================================================
grid
   18             global points
   13
   15        6
   19        2
   1000           number of cells along sides 1 and 3
   300            number of cells along sides 2 and 4
   0              sides 1 and 3 curvature: 0/1 for line/circular arc
   0              sides 1 and 3 cell spacing:
   0             sides 2 and 4 cell spacing:
   7              boundary type code for sides 1 - 4, resp.
   7
   3
   3
   0
*-------------------------------------------------------------------------
*   Side  Cell1  Cell2   #elem/cell     Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
*    1    1    1500       1           .000       297.22       0          0.
*    3    1    500        1           1.000       180.00       0          0.
*-------------------------------------------------------------------------
*                Region interface/matching
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*-------------------------------------------------------------------------
       1         1    3       3
       2         1     4      2
       3         0
       4         0
*=========================================================================
END
```

13.4 Plasma Charge Test

This is a test problem to test the Poisson solver. The geometry is a box with the potential of the *right side* set to 0V and the *left side* set to 100kV. The *top* is a Neuman BC. For the axisymmetric case (chargezr.inp), the *bottom* is the line of symmetry and is not specifiec; for the cartesian case (chargexy.inp), the bottom BC is also Neuman. Two Icarus input run files are given: dsmc.1_laplace specifies a LaPlace solution (no volume charge density) and dsmc.1_poisson specifies a Poisson solution (constant volume charge defined in the input file.



chargezr.inp

```
*---------------------------------------------------------------------
*   asterick in column 1 indicates comment card
*---------------------------------------------------------------------
*
  space charge test problem
*
*
*
*---------------------------------------------------------------------
*
control    1      -1 -- plot grid only;
*                  1 -- initialization & plot file
*
```

```
type      1             0/1 for X-Y or Z-R flow
*
plasma option    1
*
read general grid
*---------------------------------------------------------------------
*                  Region Definition
*---------------------------------------------------------------------
     1          number of regions (must be .le. 30)
     4           number of global points (must be .le.120)
*-------------------------------------
*    Global corner pt. coordinates
*  Pt.       x (m)          y (m)
*-------------------------------------
  1      0.0        0.0
  2      0.0         0.005
  3      0.01        0.005
  4      0.01        0.000
*---------------------------------------------------------------------
*           Individual Region Definitions Follow
*           --REGION NUMBERS MUST BE SEQUENTIAL--
*---------------------------------------------------------------------
*=====================================================================
region    1  <------  Inputs specific to this region follow
*
*=====================================================================
grid
   1           global points
   2
   3
   4
   100          number of cells along sides 1 and 3
   10           number of cells along sides 2 and 4
   0            sides 1 and 3 curvature: 0/1 for line/circular arc
   0            sides 1 and 3 cell spacing:
   0           sides 2 and 4 cell spacing:
   1            boundary type code for sides 1 - 4, resp.
   5
   5
   5
   3
*-------------------------------------------------------------------------
*   Side  Cell1  Cell2   elem/cell   Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
*     1    1    500     1          1.000       300.00       6          0.
      2    1    500     1          0.000       300.00       2          0.
      3    1    500     1          0.000       300.00       3          0.
      4    1    500     1          0.000       300.00       4          0.
*-------------------------------------------------------------------------
*                 Region interface/matching
*    Reg. side   reg. sides       Adj. side| Adj. reg.
```

```
*-------------------------------------------------------------------
      1         0
      2         0
      3         0
      4         0
*===================================================================================
END
*___________________________________________________________________________________
*                 END OF EXPERT INPUT FILE
*-------------------------------------------------------------------
```

chargexy.inp

```
*-------------------------------------------------------------------------
*   asterick in column 1 indicates comment card
*-------------------------------------------------------------------
*
 space charge test problem
*
*
*
*-------------------------------------------------------------------
*
control    1      -1 -- plot grid only;
*                  1 -- initialization & plot file
*
type       0              0/1 for X-Y or Z-R flow
*
plasma option    1
*
read general grid
*-------------------------------------------------------------------
*                   Region Definition
*-------------------------------------------------------------------
     1           number of regions (must be .le. 30)
     4            number of global points (must be .le.120)
*--------------------------------------
*     Global corner pt. coordinates
*  Pt.        x (m)          y (m)
*--------------------------------------
  1       0.0         0.0
  2       0.0          0.005
  3       0.01         0.005
  4       0.01         0.000
*-------------------------------------------------------------------
*            Individual Region Definitions Follow
*            --REGION NUMBERS MUST BE SEQUENTIAL--
*-------------------------------------------------------------------
*===================================================================
region    1  <------  Inputs specific to this region follow
```

```
*
*=========================================================================
grid
   1            global points
   2
   3
   4
   100           number of cells along sides 1 and 3
   50            number of cells along sides 2 and 4
   0             sides 1 and 3 curvature: 0/1 for line/circular arc
   0             sides 1 and 3 cell spacing:
   0            sides 2 and 4 cell spacing:
   5             boundary type code for sides 1 - 4, resp.
   5
   5
   5
   4
*-------------------------------------------------------------------------
*   Side  Cell1  Cell2   elem/cell   Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
     1    1     500     1          0.000        300.00       3          0.
     2    1     500     1          0.000        300.00       2          0.
     3    1     500     1          0.000        300.00       3          0.
     4    1     500     1          0.000        300.00       4          0.
*-------------------------------------------------------------------------
*                 Region interface/matching
*   Reg. side   reg. sides       Adj. side| Adj. reg.
*-------------------------------------------------------------------------
       1          0
       2          0
       3          0
       4          0
*=========================================================================
END
*_________________________________________________________________________
*                 END OF EXPERT INPUT FILE
*-------------------------------------------------------------------------
```

dsmc.1_laplace

```
# poisson test case

log file              dsmc.log

output screen          1

zero flag             5

efield flag           4

######charge density         5.e17
Te update             5
em update             1
chemistry flag        0
collision flag0
 read definition       0.2 datap
load particles        0.0
adapt flag            8000 0.25
time factor           0.001
thermal accom          0.5
output cells          1
output plasma          1
run                 1 0
```

dmsc.1_poisson

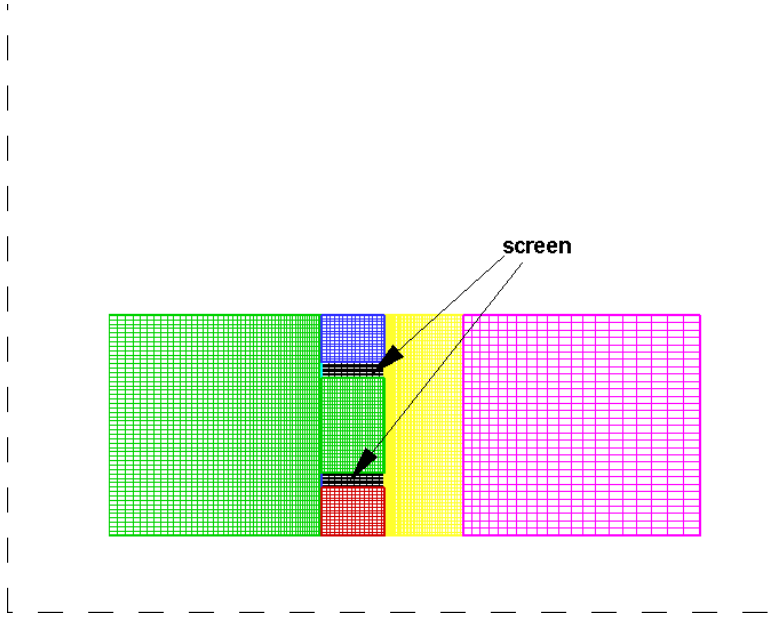
```
# poisson test case

log file              dsmc.log
 output screen         1

zero flag             5
efield flag           4
charge density         5.e17
Te update             5
em update             1
chemistry flag        0
collision flag0

read definition       0.2 datap
load particles        0.0

adapt flag            8000 0.25
time factor           0.001
thermal accom          0.5
output cells          1
output plasma          1
run                 1 0
```

surfbc

```
*
*  this file contain surface chemistry information for the
*  ntube - H2 chemistry
*       D2  D2+    D    D+   e-
*       1   2      3    4   5
*
*  variable order for each reaction:
*  (Rx type) (Species-i) (Species-r1) (Species-r2) (create prob-1)
*   (create prob 2) (degree of specular reflect) (Rx prob)
*
* For type 8:  type icode voltbc eps1 eps2 0. 0. 0.
*
3   number of material table types
*
* material 2  voltage=100kV
2  1   1.4e16
8.  1.  100000.  0.   0.0   0.  0.    0.0
*
* material 3, mirror bc (Enormal = 0), specular
3  1   1.4e16
8.  2.   0.  0.   0.0   0.  0.    0.0
*
* material 4  voltage=0V
4  1   1.4e16
8.  1.  0.  0.   0.0   0.  0.    0.0
```

13.5 Plasma Screen (Ion Accelerator)

This problem illustrates some of the electro-static boundary conditions. The problem is the flow of a charge neutral plasma injected on the left of the domain with a large negative potential applied to the right of the domain. The ions will be accelerated through the screen while the electrons are repelled; a meniscus is formed around the screen. The geometry also illustrates a gridding trick which minimized the number of regions: the screen is gridded as a region with solid walls. The upstream region is connected to 3 regions when have an interface porosity of 1.0 and 2 regions which are solid walls. A similar strategy is used with the downstream connecting region. Note the use of the type 9 electro-static boundary for material type 3 (in file surf_bc). Thus the surface potential boundary conditions for the screen are set on these regions rather on a flow domain region. Since a region's unit normals are defined as into the region, we have to flag the screen boundaries as a type 9 so that the code will reflect the normal from into the screen to into the flow domain.



file: screenz.inp

```
*-----------------------------------------------------------------------
*   asterick in column 1 indicates comment card
*-----------------------------------------------------------------------
*
 Screen - z test
*
*-----------------------------------------------------------------------
*
control    1      -1 -- plot grid only;
*                  1 -- initialization & plot file
*
type       0              0/1 for X-Y or Z-R flow
*
******options**********
*
```

```
plasma option         1
read cross_section    1
chemistry file        chem_d2
cross_section file    cross_section
surface file          surf_bc
overwrite files       1
*
read general grid
*---------------------------------------------------------------------
*---------------------------------------------------------------------
    9             number of regions (must be .le. 30)
    72            number of global points (must be .le.120)
*---------------------------------------
*     Global corner pt. coordinates
*  Pt.         x (m)          y (m)
*---------------------------------------
   1          0.00250          0.00000
   2          0.00250          0.00056
   3          0.00304          0.00056
   4          0.00304          0.00044
   5          0.00304          0.00040
   6          0.00304          0.00016
   7          0.00304          0.00012
   8          0.00304          0.00000
   9          0.00320          0.00056
  10          0.00320          0.00044
  11        0.00320          0.00040
  12          0.00320          0.00016
  13          0.00320          0.00012
  14          0.00320          0.00000
  15          0.00400          0.00168
  16          0.00400          0.00000
  17          0.00275          0.00056
  18          0.00275          0.00000
  19          0.00340          0.00056
  20          0.00340          0.00000
  21          0.00275          0.00044
  22          0.00275          0.00040
  23          0.00275          0.00016
  24          0.00275          0.00012
  25          0.00340          0.00044
  26          0.00340          0.00040
  27          0.00340          0.00016
  28          0.00340          0.00012
  29          0.00250          0.00112
  30          0.00304          0.00112
  31          0.00304          0.00100
  32          0.00304          0.00096
  33          0.00304          0.00072
  34          0.00304          0.00068
  35          0.00320          0.00112
```

```
 36        0.00320         0.00100
 37      0.00320         0.00096
 38        0.00320         0.00072
 39        0.00320         0.00068
 40        0.00400         0.00056
 41        0.00275         0.00112
 42        0.00340         0.00112
 43        0.00275         0.00100
 44        0.00275         0.00096
 45        0.00275         0.00072
 46        0.00275         0.00068
 47        0.00340         0.00100
 48        0.00340         0.00096
 49        0.00340         0.00072
 50        0.00340         0.00068
 51        0.00250         0.00168
 52        0.00304         0.00168
 53        0.00304         0.00156
 54        0.00304         0.00152
 55        0.00304         0.00128
 56        0.00304         0.00124
 57        0.00320         0.00168
 58        0.00320         0.00156
 59      0.00320         0.00152
 60        0.00320         0.00128
 61        0.00320         0.00124
 62        0.00400         0.00168
 63        0.00275         0.00056
 64        0.00340         0.00056
 65        0.00275         0.00156
 66        0.00275         0.00152
 67        0.00275         0.00128
 68        0.00275         0.00124
 69        0.00340         0.00156
 70        0.00340         0.00152
 71        0.00340         0.00128
 72        0.00340         0.00124
*------------------------------------------------------------------------
*           Individual Region Definitions Follow
*------------------------------------------------------------------------
*========================================================================
region    1  <------  Inputs specific to this region follow
*========================================================================
grid
   1           global points
   2
   63
   18
   2           number of cells along sides 1 and 3
   2            number of cells along sides 2 and 4
   0            sides 1 and 3 curvature: 0/1 for line/circular arc
```

```
   0            sides 1 and 3 cell spacing:
   0            sides 2 and 4 cell spacing:
   5            boundary type code for sides 1 - 4, resp.
   5
   5
   5
   4
*-------------------------------------------------------------------------
*  Side  Cell1  Cell2  elem/cell   Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
   1    1    20     1          1.000      300.00         0          0.
   2    1    20     1          1.000      300.00         0          0.
   3    1    20     1          1.000      300.00         0          0.
   4    1    20     1          1.000      300.00         0          0.
*-------------------------------------------------------------------------
*                Region interface/matching
*   Reg. side   reg. sides       Adj. side| Adj. reg.
*-------------------------------------------------------------------------
       1          0
       2          0
       3          0
       4          0
*=========================================================================
region    2  <------  Inputs specific to this region follow
*=========================================================================
grid
   1                18             global points
   2               63
   3
   8
   50            number of cells along sides 1 and 3
   50            number of cells along sides 2 and 4
   0            sides 1 and 3 curvature: 0/1 for line/circular arc
   3  1.03   30.   sides 1 and 3 cell spacing:
   0            sides 2 and 4 cell spacing:
   5            boundary type code for sides 1 - 4, resp.
   -51
   5
   9
   4
*-------------------------------------------------------------------------
*  Side  Cell1  Cell2  elem/cell   Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
   1    1    100    1          1.000      300.         1          0.
   2    1    100    1          1.000      300.00       2          0.
   3    1    100    1          1.000      300.         1          0.
   4    1    100    1          1.000      300.         8          1.
*-------------------------------------------------------------------------
*                Region interface/matching
*   Reg. side   reg. sides       Adj. side| Adj. reg.
*-------------------------------------------------------------------------
```

```
        1          0
        2          0
        3          0
        4          5  2 9  2 -1  2 8  2 -1  2 7
*==========================================================================
region    3  <------  Inputs specific to this region follow
*==========================================================================
grid
   7              global points
   6
   12
   13
   10              number of cells along sides 1 and 3
   10              number of cells along sides 2 and 4
   0              sides 1 and 3 curvature: 0/1 for line/circular arc
   0              sides 1 and 3 cell spacing:
   0              sides 2 and 4 cell spacing:
   5              boundary type code for sides 1 - 4, resp.
   5
   5
   5
   4
*-------------------------------------------------------------------------
*   Side  Cell1  Cell2  elem/cell   Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
    1    1     100     10          1.000       300.         3       0.0
    2    1     100     5          1.000       300.         3       0.0
    3    1     100     10          1.000       300.         3       0.0
    4    1     100     5         1.000       300.         3       0.0
*-------------------------------------------------------------------------
*                   Region interface/matching
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*
*-------------------------------------------------------------------------
        1          0
        2          0
        3          0
        4          0
*==========================================================================
region    4  <------  Inputs specific to this region follow
*==========================================================================
grid
   5              global points
  4
  10
  11
  10              number of cells along sides 1 and 3
  10              number of cells along sides 2 and 4
   0              sides 1 and 3 curvature: 0/1 for line/circular arc
   0              sides 1 and 3 cell spacing:
   0              sides 2 and 4 cell spacing:
```

```
   5            boundary type code for sides 1 - 4, resp.
   5
   5
   5
   4
*-------------------------------------------------------------------------
*   Side  Cell1  Cell2  elem/cell   Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
    1    1     100    10          1.000      300.         3       0.0
    2    1     100    5          1.000      300.         3       0.0
    3    1     100    10          1.000      300.         3       0.0
    4    1     100    5          1.000      300.         3       0.0
*-------------------------------------------------------------------------
*                 Region interface/matching
*              Number adj.
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*-------------------------------------------------------------------------
        1          0
        2          0
        3          0
        4          0
*=========================================================================
region    5 <------  Inputs specific to this region follow
*=========================================================================
grid
   14            global points
   9
   64
   20
  40             number of cells along sides 1 and 3
  60             number of cells along sides 2 and 4
   0             sides 1 and 3 curvature: 0/1 for line/circular arc
   2  1.03   30.   sides 1 and 3 cell spacing:
   0             sides 2 and 4 cell spacing:
   5             boundary type code for sides 1 - 4, resp.
   9
   5
   7
   3
*-------------------------------------------------------------------------
*   Side  Cell1  Cell2  elem/cell   Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
    1    1     100    1          1.000      300.00       1         0.
    2    1     100    1          1.000      300.         8       1.0
    3    1     100    1          1.000      300.00       1         0.
*-------------------------------------------------------------------------
*                 Region interface/matching
*              Number adj.
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*-------------------------------------------------------------------------
        1          0
```

```
      2         5  4 7  4 -1  4 8  4 -1  4 9
      3         0
      4         1    2  6
*-------------------------------------------------------------------------
*=========================================================================
region    6 <------  Inputs specific to this region follow
*=========================================================================
grid
   20             global points
   64
   40
   16
   20             number of cells along sides 1 and 3
   30             number of cells along sides 2 and 4
   0              sides 1 and 3 curvature: 0/1 for line/circular arc
   2 1.04  50.    sides 1 and 3 cell spacing:
   0              sides 2 and 4 cell spacing:
   5              boundary type code for sides 1 - 4, resp.
   7
   5
   5
   3
*-------------------------------------------------------------------------
*   Side  Cell1  Cell2  elem/cell   Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
    1     1      200      1         1.000       300.         1          0.
    3     1      200      1         1.000       300.         1          0.
    4     1      220      1         0.000       300.         4          0.
*-------------------------------------------------------------------------
*                 Region interface/matching
*              Number adj.
*   Reg. side   reg. sides       Adj. side| Adj. reg.
*-------------------------------------------------------------------------
      1         0
      2         1   4 5
      3         0
      4         0
*=========================================================================
*=========================================================================
region    7 <------  Inputs specific to this region follow
*=========================================================================
grid
   8              global points
   7
   13
   14
   15             number of cells along sides 1 and 3
   15             number of cells along sides 2 and 4
   0              sides 1 and 3 curvature: 0/1 for line/circular arc
   0              sides 1 and 3 cell spacing:
   0              sides 2 and 4 cell spacing:
```

```
   5            boundary type code for sides 1 - 4, resp.
   7
   5
   7
   2
*-------------------------------------------------------------------------
*  Side  Cell1  Cell2  elem/cell   Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
   1    1     100    1          1.000      300.         1          0.
   3    1     100    1          1.000      300.         8          0.
*-------------------------------------------------------------------------
*       |-----> Only need if IVN > 0; then supply IVN pairs of (IVR,IVS)
*             Number adj.
*   Reg. side   reg. sides       Adj. side| Adj. reg.
*-------------------------------------------------------------------------
       1          0
       2          1  4  2
       3          0
       4          1  2  5
*=========================================================================
*=========================================================================
region    8  <------  Inputs specific to this region follow
*=========================================================================
grid
   6            global points
   5
   11
   12
   25            number of cells along sides 1 and 3
   25            number of cells along sides 2 and 4
   0             sides 1 and 3 curvature: 0/1 for line/circular arc
   0             sides 1 and 3 cell spacing:
   0             sides 2 and 4 cell spacing:
   5             boundary type code for sides 1 - 4, resp.
   7
   5
   7
   2
*-------------------------------------------------------------------------
*  Side  Cell1  Cell2  elem/cell   Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
   1    1     100    1          1.000      300.         8          0.
   3    1     100    1          1.000      300.         8          0.
*-------------------------------------------------------------------------
*                Region interface/matching
*             Number adj.
*   Reg. side   reg. sides       Adj. side| Adj. reg.
*-------------------------------------------------------------------------
       1          0
       2          1  4  2
       3          0
```

```
      4         1  2  5
*=========================================================================
*=========================================================================
region    9  <------  Inputs specific to this region follow
*=========================================================================
grid
   4              global points
   3
   9
   10
   15             number of cells along sides 1 and 3
   15             number of cells along sides 2 and 4
   0              sides 1 and 3 curvature: 0/1 for line/circular arc
   0              sides 1 and 3 cell spacing:
   0              sides 2 and 4 cell spacing:
   5              boundary type code for sides 1 - 4, resp.
   7
   5
   7
   2
*-------------------------------------------------------------------------
*   Side  Cell1  Cell2  elem/cell   Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
    1    1     100     1          1.000       300.          8          0.
    3    1     100     1          1.000       300.          1          0.
*-------------------------------------------------------------------------
*                 Region interface/matching
*              Number adj.
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*-------------------------------------------------------------------------
       1          0
       2          1  4  2
       3          0
       4          1  2  5
*=========================================================================
END
************************End of Input**********************************
```

file: surf_bc

```
*
*  this file contain surface chemistry information for the
*  ntube - H2 chemistry
*       D2  D    D2+    D+  Fe-    E
*       1   2    3    4     5       6
*
*  variable order for each reaction:
*  (Rx type) (Species-i) (Species-r1) (Species-r2) (create prob-1)
*   (create prob 2) (degree of specular reflect) (Rx prob)
*
* For type 8:  type icode voltbc eps1 eps2 0. 0. 0.
*
8   number of material table types
*
* material 1 sym. BC -- voltage=0, specular side 1
1 1  1.4e16
8   2. 0.0  1.0  0.0   0.  0.    0.0
*
* material 5 sym. BC -- voltage=0, specular side 3
5 1  1.4e16
8   2. .0  0.0  0.0   0.  0.    0.0
*****8   2. .0  3.0  0.0   0.  0.    0.0
* material 2, old inlet surface file
2  6   1.4e16
1.  1.   1.  0.   0.0   0.  1.    1.0
1.  2.   2.  0.   0.0   0.  1.    1.0
1.  3.   3.  0.   0.0   0.  1.    1.0
1.  4.   4.  0.   0.0   0.  1.    1.0
1.  5.   5.  0.   0.0   0.  1.    1.0
8.  1.   0.  0.   0.0   0.  0.    0.0
*
* material 3, screen -- voltage bc,
3  4   1.4e16
1.  2.   2.  0.   0.0   0.  0.    1.0
1.  4.   2.  0.   1.0   0.  0.    1.0
1.  5.   5.  0.   0.0   0.  0.    1.0
8.  9.   0.  0.   0.0   0.  0.    0.0
*
* material 4,  ions go into target.
4  4   1.4e16
1.  2.   2.  0.   0.0   0.  0.    1.0
1.  4.   4.  0.   0.0   0.  0.    1.0
1   5.   5.  0.   0.0   0.  0.    1.0
8.  1.   -10000.  0.   0.0   0.  0.    0.0
* material 6,  all particles stick -- inlet bc
6  3   1.4e16
1.  3.   3.  0.   0.0   0.  0.    1.0
1.  4.   4.  0.   0.0   0.  0.    1.0
1   5.   5.  0.   0.0   0.  0.    1.0
* material 7 sym. BC -- voltage=0, specular sSide 1
```

```
7 1  1.4e16
8   1. 0.0  1.0  0.0   0.  0.    0.0
*
*
* material 8, screen -- with NO voltage bc,
8  3   1.4e16
1.  2.   2.  0.   0.0   0.  0.    1.0
1.  4.   2.  0.   1.0   0.  0.    1.0
1.  5.   5.  0.   0.0   0.  0.    1.0
```

13.6 Micro-Gyroscope

This problem illustrates the use of a 'test point' to monitor the pressure/density at a given location in the flowfield and also the rotating boundary condition. Although this simulations is axisymmetric, one surface is rotating at a given rotational speed, W. Thus, when a molecule hits this surface, an 'out-of-plane' or V-theta velocity is rw, r is the local radial distance. The domain consists of 2 regions along the R axis: the first region is bounded by the centerline, a fixed wall, and the rotating wall. The second region is bounded by 2 fixed walls and a line of symmetry. This system is closed.

file: gyro.inp

```
*-------------------------------------------------------------------------
*   asterick in column 1 indicates comment card
*-------------------------------------------------------------------------
*
 micro-gyro --- base case
*
*
*-------------------------------------------------------------------------
*       options section
*-------------------------------------------------------------------------
*
control    1          -1 -- plot grid only;
*                      1 -- initialization & plot file
*
type             1       0/1 for X-Y or Z-R flow
*
cell weight    4
*-------------------------------------------------------------------------
read general grid
*
    2           number of regions
    7           number of global points
*-------------------------------------
*     Global corner pt. coordinates
*  Pt.        z (m)          r(m)
*-------------------------------------
  1         0.0              0.0
  2         0.000             500.e-6
  3         0.000             750.e-6
  4         1.e-6            0.00
  5         1.e-6            500e-6
  6         1.e-6            750.e-6
  7         0.5e-6             500.e-6
*
read test points -1
  1    7
*
```

```
*========================================================================
region   1 <------  Inputs specific to this region follow
*========================================================================
grid
   1            global points
   2
   5
   4
   10            number of cells along sides 1 and 3
   225             number of cells along sides 2 and 4
   0            sides 1 and 3 curvature: 0/1 for line/circular arc
   0            sides 1 and 3 cell spacing:
   0            sides 2 and 4 cell spacing:
   1            boundary type code for sides 1 - 4, resp.
   5
   7
   5
   2
*------------------------------------------------------------------------
*   Side  Cell1  Cell2 #elem/cell    Spec. refl.   Temp. K    Material#    Value
*------------------------------------------------------------------------
   2    1    300      1          0.000      300.       0          0.
   4    1    700      1          0.000      300.       1          0.0
*------------------------------------------------------------------------
*                 Region interface/matching
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*------------------------------------------------------------------------
       1          0
       2          0
       3          1              1      2
       4          0
*========================================================================
region   2 <------  Inputs specific to this region follow
*========================================================================
grid
   2            global points
   3
   6
   5
   10            number of cells along sides 1 and 3
   100             number of cells along sides 2 and 4
   0            sides 1 and 3 curvature: 0/1 for line/circular arc
   0            sides 1 and 3 cell spacing:
   0            sides 2 and 4 cell spacing:
   7            boundary type code for sides 1 - 4, resp.
   5
   5
   5
   3
*------------------------------------------------------------------------
*   Side  Cell1  Cell2  #elem/cell   Spec. refl.   Temp. K    Material#    Value
```

```
*-----------------------------------------------------------------------
   2    1    300       1         0.000      300.      0         0.
   3    1    300       1         0.000      300.      0         0.
   4    1    300       1         1.000      300.      0         0.0
*-----------------------------------------------------------------------
*                 Region interface/matching
*               Number adj.
*    Reg. side   reg. sides       Adj. side| Adj. reg.
*-----------------------------------------------------------------------
        1          1              3       1
        2          0
        3          0
        4          0
*-----------------------------------------------------------------------
END                  END OF EXPERT INPUT FILE
*-----------------------------------------------------------------------
```

file: inlet

```
*
*   initial conditions for the micro-gyro
*
*     N2 species
*
1 number of tables
*
0   -----  flag to specify initial conditions
0.1212e+25    0.0    0.0     300.   300.   300.    1.
*
```

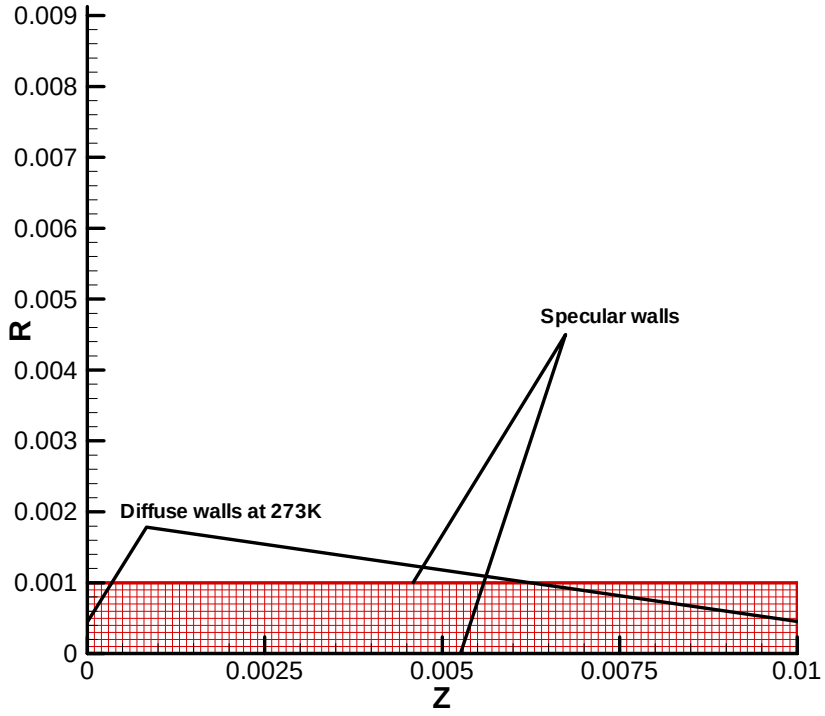
file: surfbc

```
*
*      N2
*      1    2    3
*
*  variable order for each reaction:
*
*
1    number of material table types
*
1 1 1.0
-7. 00.  0.0    16666.7   0.0   0.0   0.0   0.0
```

13.7 Collisional Test in a Closed Box

Isothermal flow of nitrogen in a closed box

Purpose. While this test case does not exercise any of the sophisticated options of Icarus it is particularly useful for validation/verification purposes. The flowfield is a two-dimensional box with two specular and two diffuse walls, divided into 1000 cells (100 across x and 10 across y). For a pressure of 100mTorr the number density is such that the mean free path is a third of the cell size. For a timestep of 10-7 all the DSMC requirements for an accurate calculation are satisfied. The test case can be ran either collisionless (by inhibiting collisions) or with collisions. In the first case the heat and number flux to the diffuse walls can be calculated (surface files) and compared with the predictions of collisionless gas theory (see Bird 1994 chapter 7). In the latter case the ability of the code to achieve equilibration between the internal and translational modes, and the correct heat and mass fluxes to the walls can be verified. The collision frequency as predicted by the code can be also calculated under conditions of perfect equilibrium. All these properties can also be calculated analytically (see Bird, ref. 11.1, Chapter 4) and compared with the predictions of Icarus. Comparisons made by the authors indicate agreement better than 1%.



Input File

```
*-------------------------------------------------------------------------
*   asterick in column 1 indicates comment card
*-------------------------------------------------------------------------
*
100mTorr/N2
*
*
*-------------------------------------------------------------------------
*       options section
*-------------------------------------------------------------------------
*
control    1     -1 -- plot grid only;
*                   1 -- initialization & plot file
*
type             0       0/1 for X-Y or Z-R flow
*
cell weight    0
*-------------------------------------------------------------------------
read general grid
*
    1           number of regions
    4           number of global points
*--------------------------------------
*     Global corner pt. coordinates
*  Pt.        z (m)          r(m)
*--------------------------------------
1  .0   .0
2  .0   .001
3  .01  .001
4  .01  .0
*-------------------------------------------------------------------
*            Individual Region Definitions Follow
*            --REGION NUMBERS MUST BE SEQUENTIAL--
*-------------------------------------------------------------------
*===================================================================================
region   1  <------  Inputs specific to this region follow
*===================================================================================
grid
   1             global points
   2
   3
   4
   100        number of cells along sides 1 and 3
   10         number of cells along sides 2 and 4
   0             sides 1 and 3 curvature: 0/1 for line/circular arc
   0             sides 1 and 3 cell spacing:
   0             sides 2 and 4 cell spacing:
   5           boundary type code for sides 1 - 4, resp.
   5
   5
```

```
   5
   4
*-------------------------------------------------------------------
*  Side  Cell1  Cell2  #elem/cell   Spec. refl.   Temp. K   Material#    Value
*-------------------------------------------------------------------
   1    1    100      1          1.000       273.00       0          0.
   2    1    100      1           .000       273.00       0          0.
   3    1    100      1          1.000       273.00       0          0.
   4    1    100      1           .000       273.00       0          0.
*-------------------------------------------------------------------
*                Region interface/matching
*   Reg. side   reg. sides       Adj. side| Adj. reg.
*-------------------------------------------------------------------
       1          0
       2          0
       3          0
       4          0
*===================================================================================
*-------------------------------------------------------------------
END                 END OF EXPERT INPUT FILE
*-------------------------------------------------------------------
```

Inlet File

```
*
_*   freestream inlet condition for the N2 box relaxation
*
*     N2 species
*
1 number of tables
*
0   -----  flag to specify freestream conditions
3.537156e21  0.    0.0     273.   273.   273.    1.
*
```

Species File

```
****************************************
_*       new species data file         *
****************************************
*
1             number of species
*
3             internal structure of most complex molecule:
*                  3-monatomic, 4-rotation, 5-rotat. + vibrat.
*
0             # of chem. rx. (from file chem)
*
*
*-------------------------------------------------------------------------------------------------------------
*  ID
```

```
        * Mwt    Mol. mass   Diam.   #Rot.Deg.    Rot.Rel. #Vit. Deg. Vib. Rel. Vib.Temp. specie wt. charge  ome-
ga  tref  alpha
        *          (kg)       (m)     Freedom      Coll. #    Freedom    Coll. #     (K)
        *-------------------------------------------------------------------------------------------------------------
         N2
         28.0   4.65E-26  4.11E-10      2.           5.       50.       5.       3371.      1.0      0.0     0.74    273.   1.0
        *
        END     MUST have this line as last input line.....
```

13.8 MBF Expansion Chamber (reference paper 12.3)

The problem illustrates the use of the input from a Navier-Stokes code to provide the boundary plane at the nozzle throat. Also, the collision limiter logic, used to limit the number of test particle collisions was developed for this problem.

- Input Gases: He & C3H6O

- Chemical Species:

	Mwt	Mass	VHS diameter
He	4.004 gm/gmole	6.648 x 10-27 kg	2.19 x 10-10 m
C3H6O	70.91 gm/gmole	9.64 x 10-26 kg	6.67 x 10-10 m

use a mixture viscosity coeficient of 0.658531 @ 273 K

- Boundary conditions:
  - inlet: sonic choked boundary
    Mole fractions: He= 1.0C3H6O= 0.0
  - outlet: nonreentrant boundary (perfect vacuum pump)

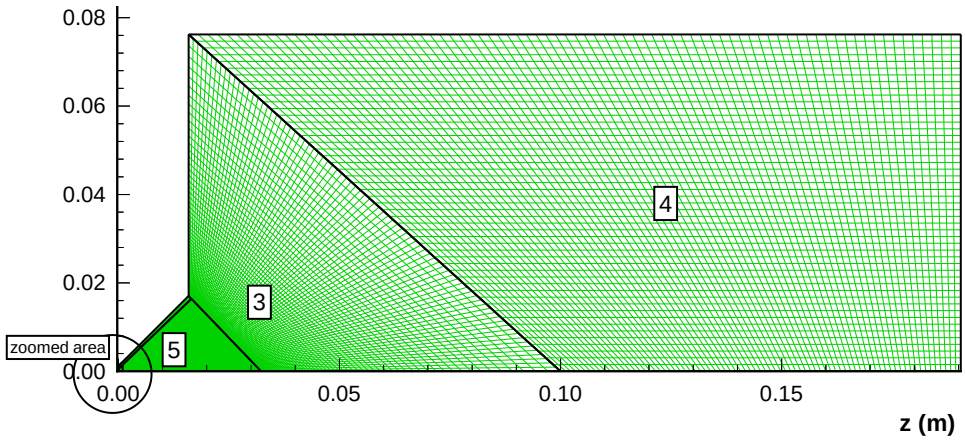
- Surface Boundary Conditions:
  - 100% thermal accommodation
  - 100% diffuse surface reaction
  - Temperature of all surfaces = 232.31 K

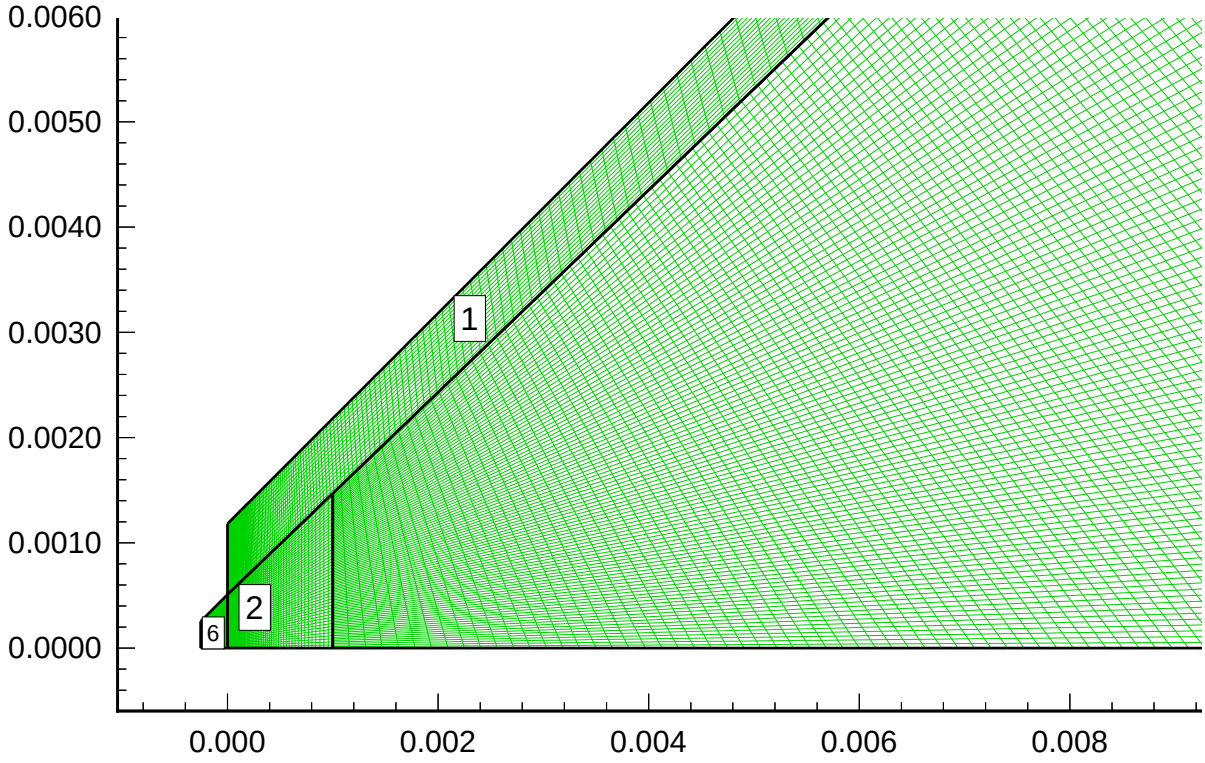
- Surface Chemistry:
  no reactions

- Output:
  - pressure, velocity, temperature and species distribution
  - transient flowfield results

- Reference:

T. J. Bartel et. al., "DSMC Simulation of Nozzle Expansion Flow Fields," AIAA 94-2047, 6th AIAA/ASME Joint Thermophysics & Heat Transfer Conference, Colorado Springs, CO, 1994.





input file:

```
*-----------------------------------------------------------------------
*   asterick in column 1 indicates comment card
*-----------------------------------------------------------------------
*
 MBF - He-Acetone    transient simulation
*
*
*-----------------------------------------------------------------------
*
control    1      -1 -- plot grid only;
*                  1 -- initialization & plot file
*
type       1              0/1 for X-Y or Z-R flow
*
cell weight           -4
expansion radius wt     5.08e-4
*
*
read general grid
*-----------------------------------------------------------------------
*                    Region Definition
*-----------------------------------------------------------------------
    6           number of regions (must be .le. 30)
    30           number of global points (must be .le.120)
```

```
*--------------------------------------
*    Global corner pt. coordinates
*  Pt.       z (m)          r(m)
*--------------------------------------
   1      0.000          0.0
   2      1.5875e-2      0.0
   3      3.2258e-2      0.0
   4      1.905e-1       0.0
   5      0.0           5.08e-4
   6      1.65215e-2     1.63833e-2
   7      0.00          1.1811e-3
   8      1.5875e-2      1.7056e-2
   9      1.5875e-2      7.62e-2
  10      1.905e-1       7.62e-2
  11      0.01           0.01
  12      0.01           0.0005
  13      0.005          0.0005
  14     -0.00049        0.0
  15     -0.00049        0.0005
  16      0.002          0.00
  17      0.00           0.002
  18      0.015          0.03
  19      0.03           0.02
  20      0.1           0.0
  21      0.001          0.0
  22      0.001          1.46892e-3
  23      0.01           0.00
*  24     0.01           1.01207e-2
  24      0.01           1.0508e-2
  25      0.01           1.1181e-2
  26      1.5875e-2      0.0
  27     -2.54e-4        0.0
  28     -2.54e-4        2.54e-4
  29      0.012          0.0
  30      0.012          1.31811e-2
*--------------------------------------
*=========================================================================
region    1  <------  Inputs specific to this region follow
*=========================================================================
grid
   5             global points
   7
   8
   6
 200              number of cells along sides 1 and 3
  20              number of cells along sides 2 and 4
   0             sides 1 and 3 curvature:: 0/1 for line/circular arc
   2  1.03  40     sides 1 and 3 cell spacing:
   0             sides 2 and 4 cell spacing:
   7             boundary type code for sides 1 - 4, resp.
   5
   5
```

```
   7
   2            number of BC entries
*-------------------------------------------------------------------
*   Side  Cell1  Cell2  elem/cell    Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------
    2    1     100    1           0.000       300.00       0          0.
    3    1     200    1           0.000       300.00       0          0.
*-------------------------------------------------------------------
*
*-------------------------------------------------------------------
*-------------------------------------------------------------------
*                Region interface/matching
*    Reg. side   reg. sides       Adj. side  Adj. reg.
*-------------------------------------------------------------------
*-------------------------------------------------------------------
       1         2             3    5    3  2
       2         0
       3         0
       4         1             1    3
*===================================================================
region    2  <------  Inputs specific to this region follow
*===================================================================
grid
   1            global points
   5
  22
  21
  60            number of cells along sides 1 and 3
  50            number of cells along sides 2 and 4
   0            sides 1 and 3 curvature: 0/1 for line/circular arc
   2  1.04  50     sides 1 and 3 cell spacing:
   0            sides 2 and 4 cell spacing:
   1            boundary type code for sides 1 - 4, resp.
   7
   7
   7
   0            number of BC entries
*-------------------------------------------------------------------
*   Side  Cell1  Cell2 elem/cell    Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------
*
*-------------------------------------------------------------------
*-------------------------------------------------------------------
*                Region interface/matching
*    Reg. side   reg. sides       Adj. side  Adj. reg.
*-------------------------------------------------------------------
*-------------------------------------------------------------------
       1         0
       2         1             4  6
       3         1             1  1
       4         1             2  5
```

```
*========================================================================
region    3  <------  Inputs specific to this region follow
*========================================================================
grid
   8              global points
   9
  20
   3
  80              number of cells along sides 1 and 3
  60              number of cells along sides 2 and 4
   0              sides 1 and 3 curvature: 0/1 for line/circular arc
   0              sides 1 and 3 cell spacing:
   2  1.04  50     sides 2 and 4 cell spacing:
   7              boundary type code for sides 1 - 4, resp.
   5
   7
   1
   1              number of BC entries
*------------------------------------------------------------------------
*   Side  Cell1  Cell2 elem/cell     Spec. refl.   Temp. K    Material#    Value
*------------------------------------------------------------------------
   2      1    100      1            0.0          300.        0           0.
*------------------------------------------------------------------------
*
*------------------------------------------------------------------------
*------------------------------------------------------------------------
*                 Region interface/matching
*    Reg. side   reg. sides       Adj. side  Adj. reg.
*------------------------------------------------------------------------
*------------------------------------------------------------------------
       1          2              4  5  4   1
       2          0
       3          1              2        4
       4          0
*========================================================================
region    4  <------  Inputs specific to this region follow
*========================================================================
grid
  20              global points coinciding w/ region corner points 1 - 4, resp.
   9
  10
   4
  80              number of cells along sides 1 and 3
  50              number of cells along sides 2 and 4
   0              sides 1 and 3 curvature: 0/1 for line/circular arc
   0              sides 1 and 3 cell spacing:
   0              sides 2 and 4 cell spacing:
   1              boundary type code for sides 1 - 4, resp.
   7
   5
   11
   1             number of BC entries
*------------------------------------------------------------------------
```

```
*   Side  Cell1  Cell2  elem/cell   Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
    3     1      100       1          0.000       300.00        0          0.
*-------------------------------------------------------------------------
*
*-------------------------------------------------------------------------
*-------------------------------------------------------------------------
*                 Region interface/matching
*    Reg. side   reg. sides       Adj. side  Adj. reg.
*-------------------------------------------------------------------------
*-------------------------------------------------------------------------
       1          0
       2          1           3   3
       3          0
       4          0
*=========================================================================
region    5 <------  Inputs specific to this region follow
*=========================================================================
grid
   21              global points
   22
    6
    3
  200               number of cells along sides 1 and 3
  100               number of cells along sides 2 and 4
    0               sides 1 and 3 curvature: 0/1 for line/circular arc
    0               sides 1 and 3 cell spacing:
    0               sides 2 and 4 cell spacing:
    1               boundary type code for sides 1 - 4, resp.
    7
    7
    7
    0               number of surface bc
*-------------------------------------------------------------------------
*   Side  Cell1  Cell2  elem/cell    Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
*
*-------------------------------------------------------------------------
*-------------------------------------------------------------------------
*                 Region interface/matching
*    Reg. side   reg. sides       Adj. side  Adj. reg.
*-------------------------------------------------------------------------
*-------------------------------------------------------------------------
       1          0
       2          1          4   2
       3          1          1   1
       4          1          1   3
*=========================================================================
region    6 <------  Inputs specific to this region follow
*=========================================================================
grid
   27              global points
```

```
  28
   5
   1
  60            number of cells along sides 1 and 3
  50            number of cells along sides 2 and 4
   0            sides 1 and 3 curvature: 0/1 for line/circular arc
   0            sides 1 and 3 cell spacing:
   0            sides 2 and 4 cell spacing:
   1            boundary type code for sides 1 - 4, resp.
 -31
   5
   7
   1            number of BC entries
*-------------------------------------------------------------------------
*   Side  Cell1  Cell2  elem/cell    Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
    3     1      250      1          0.000       300.00        0          0.
*-------------------------------------------------------------------------
*
*-------------------------------------------------------------------------
*-------------------------------------------------------------------------
*                 Region interface/matching
*    Reg. side   reg. sides       Adj. side  Adj. reg.
*-------------------------------------------------------------------------
*-------------------------------------------------------------------------
       1          0
       2          0
       3          0
       4          1          2    2
*-------------------------------------------------------------------------
END                END OF EXPERT INPUT FILE
*-------------------------------------------------------------------------
```

inlet file:

```
*
1        table for the MBF nozzle(INCA-M=1.05:plane at 2.53429e-4m)-file:inlet.bc
1   1   69    3      table #,  # of table entries, BC type
*
*   r         number density    Vz       Vr      Tt         Tr           Tv     fraction species 1   2
*      units are MKS
 0.000000E+00  0.610425E+26 941.7240   0.0000 0.2323E+03 0.2323E+03 0.2323E+03    0.999      .001
 0.146677E-04  0.610425E+26 941.7240   0.0000 0.2323E+03 0.2323E+03 0.2323E+03    0.999      .001
 0.284893E-04  0.610423E+26 941.7250   0.0002 0.2323E+03 0.2323E+03 0.2323E+03    0.999      .001
 0.415138E-04  0.610423E+26 941.7260   0.0004 0.2323E+03 0.2323E+03 0.2323E+03    0.999      .001
 0.537871E-04  0.610422E+26 941.7270   0.0006 0.2323E+03 0.2323E+03 0.2323E+03    0.999      .001
 0.653527E-04  0.610420E+26 941.7290   0.0008 0.2323E+03 0.2323E+03 0.2323E+03    0.999      .001
 0.762515E-04  0.610420E+26 941.7290   0.0009 0.2323E+03 0.2323E+03 0.2323E+03    0.999      .001
 0.865219E-04  0.610420E+26 941.7280   0.0008 0.2323E+03 0.2323E+03 0.2323E+03    0.999      .001
 0.962003E-04  0.610423E+26 941.7250   0.0003 0.2323E+03 0.2323E+03 0.2323E+03    0.999      .001
 0.105321E-03  0.610426E+26 941.7190  -0.0008 0.2323E+03 0.2323E+03 0.2323E+03    0.999      .001
 0.113916E-03  0.610434E+26 941.7100  -0.0029 0.2323E+03 0.2323E+03 0.2323E+03    0.999      .001
```

0.122016E-03	0.610443E+26	941.6970	-0.0060	0.2323E+03	0.2323E+03	0.2323E+03	0.999	.001
0.129649E-03	0.610453E+26	941.6800	-0.0103	0.2323E+03	0.2323E+03	0.2323E+03	0.999	.001
0.136843E-03	0.610467E+26	941.6630	-0.0153	0.2323E+03	0.2323E+03	0.2323E+03	0.999	.001
0.143622E-03	0.610479E+26	941.6470	-0.0207	0.2323E+03	0.2323E+03	0.2323E+03	0.999	.001
0.150012E-03	0.610486E+26	941.6370	-0.0253	0.2323E+03	0.2323E+03	0.2323E+03	0.999	.001
0.156033E-03	0.610486E+26	941.6390	-0.0278	0.2323E+03	0.2323E+03	0.2323E+03	0.999	.001
0.161709E-03	0.610474E+26	941.6600	-0.0262	0.2323E+03	0.2323E+03	0.2323E+03	0.999	.001
0.167058E-03	0.610443E+26	941.7070	-0.0182	0.2323E+03	0.2323E+03	0.2323E+03	0.999	.001
0.172100E-03	0.610387E+26	941.7910	-0.0011	0.2323E+03	0.2323E+03	0.2323E+03	0.999	.001
0.176852E-03	0.610298E+26	941.9230	0.0285	0.2323E+03	0.2323E+03	0.2323E+03	0.999	.001
0.181332E-03	0.610167E+26	942.1120	0.0741	0.2322E+03	0.2322E+03	0.2322E+03	0.999	.001
0.185555E-03	0.609987E+26	942.3720	0.1400	0.2322E+03	0.2322E+03	0.2322E+03	0.999	.001
0.189536E-03	0.609747E+26	942.7140	0.2307	0.2321E+03	0.2321E+03	0.2321E+03	0.999	.001
0.193289E-03	0.609437E+26	943.1540	0.3517	0.2320E+03	0.2320E+03	0.2320E+03	0.999	.001
0.196827E-03	0.609050E+26	943.7030	0.5090	0.2319E+03	0.2319E+03	0.2319E+03	0.999	.001
0.203309E-03	0.607992E+26	945.1890	0.9614	0.2317E+03	0.2317E+03	0.2317E+03	0.999	.001
0.206276E-03	0.607298E+26	946.1510	1.2733	0.2315E+03	0.2315E+03	0.2315E+03	0.999	.001
0.209074E-03	0.606479E+26	947.2800	1.6554	0.2313E+03	0.2313E+03	0.2313E+03	0.999	.001
0.211713E-03	0.605524E+26	948.5890	2.1188	0.2311E+03	0.2311E+03	0.2311E+03	0.999	.001
0.214203E-03	0.604427E+26	950.0980	2.6759	0.2308E+03	0.2308E+03	0.2308E+03	0.999	.001
0.216552E-03	0.603180E+26	951.8240	3.3405	0.2305E+03	0.2305E+03	0.2305E+03	0.999	.001
0.218769E-03	0.601783E+26	953.7870	4.1280	0.2301E+03	0.2301E+03	0.2301E+03	0.999	.001
0.220861E-03	0.600232E+26	956.0070	5.0556	0.2297E+03	0.2297E+03	0.2297E+03	0.999	.001
0.222836E-03	0.598528E+26	958.4950	6.1421	0.2292E+03	0.2292E+03	0.2292E+03	0.999	.001
0.224701E-03	0.596664E+26	961.2550	7.4077	0.2287E+03	0.2287E+03	0.2287E+03	0.999	.001
0.226462E-03	0.594633E+26	964.2800	8.8731	0.2281E+03	0.2281E+03	0.2281E+03	0.999	.001
0.228126E-03	0.592422E+26	967.5460	10.5587	0.2275E+03	0.2275E+03	0.2275E+03	0.999	.001
0.229699E-03	0.590004E+26	971.0140	12.4847	0.2268E+03	0.2268E+03	0.2268E+03	0.999	.001
0.231185E-03	0.587356E+26	974.6250	14.6690	0.2260E+03	0.2260E+03	0.2260E+03	0.999	.001
0.232591E-03	0.584444E+26	978.3060	17.1268	0.2253E+03	0.2253E+03	0.2253E+03	0.999	.001
0.233921E-03	0.581242E+26	981.9660	19.8690	0.2245E+03	0.2245E+03	0.2245E+03	0.999	.001
0.235181E-03	0.577728E+26	985.5060	22.8939	0.2237E+03	0.2237E+03	0.2237E+03	0.999	.001
0.236373E-03	0.573890E+26	988.8250	26.1895	0.2230E+03	0.2230E+03	0.2230E+03	0.999	.001
0.237504E-03	0.569716E+26	991.8270	29.7463	0.2224E+03	0.2224E+03	0.2224E+03	0.999	.001
0.238576E-03	0.565195E+26	994.4260	33.5554	0.2218E+03	0.2218E+03	0.2218E+03	0.999	.001
0.239593E-03	0.560317E+26	996.5400	37.6030	0.2213E+03	0.2213E+03	0.2213E+03	0.999	.001
0.240560E-03	0.555077E+26	998.0970	41.8680	0.2210E+03	0.2210E+03	0.2210E+03	0.999	.001
0.241479E-03	0.549471E+26	999.0400	46.3152	0.2207E+03	0.2207E+03	0.2207E+03	0.999	.001
0.242354E-03	0.543508E+26	999.3340	50.8990	0.2206E+03	0.2206E+03	0.2206E+03	0.999	.001
0.243188E-03	0.537218E+26	998.9510	55.5788	0.2206E+03	0.2206E+03	0.2206E+03	0.999	.001
0.243983E-03	0.530613E+26	997.8610	60.3215	0.2208E+03	0.2208E+03	0.2208E+03	0.999	.001
0.244743E-03	0.523698E+26	996.0320	65.0949	0.2210E+03	0.2210E+03	0.2210E+03	0.999	.001
0.245471E-03	0.516481E+26	993.4200	69.8661	0.2215E+03	0.2215E+03	0.2215E+03	0.999	.001
0.246168E-03	0.508962E+26	989.9740	74.6020	0.2221E+03	0.2221E+03	0.2221E+03	0.999	.001
0.246838E-03	0.501135E+26	985.6220	79.2665	0.2229E+03	0.2229E+03	0.2229E+03	0.999	.001
0.247482E-03	0.492995E+26	980.2630	83.8187	0.2238E+03	0.2238E+03	0.2238E+03	0.999	.001
0.248103E-03	0.484526E+26	973.7540	88.2192	0.2250E+03	0.2250E+03	0.2250E+03	0.999	.001
0.248703E-03	0.475739E+26	965.8640	92.4555	0.2264E+03	0.2264E+03	0.2264E+03	0.999	.001
0.249285E-03	0.466683E+26	956.2080	96.5942	0.2281E+03	0.2281E+03	0.2281E+03	0.999	.001
0.249850E-03	0.457380E+26	944.3170	100.7240	0.2302E+03	0.2302E+03	0.2302E+03	0.999	.001
0.250400E-03	0.447682E+26	929.7660	104.6890	0.2327E+03	0.2327E+03	0.2327E+03	0.999	.001

```
0.250938E-03  0.437375E+26 911.8630 107.9540 0.2358E+03 0.2358E+03 0.2358E+03    0.999       .001
0.251465E-03  0.426346E+26 889.0870 109.7260 0.2395E+03 0.2395E+03 0.2395E+03    0.999       .001
0.251982E-03  0.414573E+26 858.6020 108.9840 0.2439E+03 0.2439E+03 0.2439E+03    0.999       .001
0.252493E-03  0.402026E+26 815.4470 103.9530 0.2494E+03 0.2494E+03 0.2494E+03    0.999       .001
0.252998E-03  0.388550E+26 750.9500  90.3279 0.2560E+03 0.2560E+03 0.2560E+03    0.999       .001
0.253500E-03  0.374430E+26 649.8740  57.8191 0.2628E+03 0.2628E+03 0.2628E+03    0.999       .001
0.254000E-03  0.311123E+26   0.0000   0.0000 0.3000E+03 0.3000E+03 0.3000E+03    0.999       .001
```

Icarus input file:

```
# MBF - He-Acetone (0.001)  t1

log file   dsmc.log

output screen100

zero flag20


read def  1.0 datap

adapt flag            200 0.25
time factor        0.001

output cell           1000
output surf           5000

run                  20000 0
```

13.9 NO Nozzle Expansion and Data Comparison (reference paper 12.2)

This problem illustrates how the choice of grid regions and cell clustering can be chosen to improve the accurary of the simulation.

- Input Gases: NO

- Boundary conditions:
  inlet: 25 torr pulsed valve (radial inlet)
  outlet: vacuum

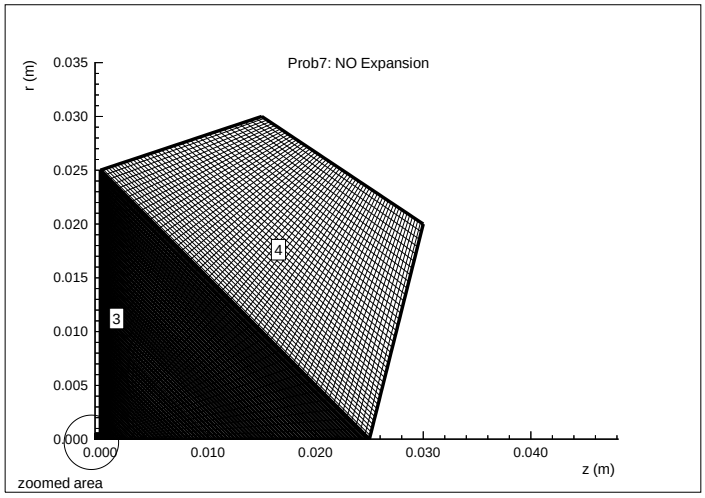
- Surface Boundary Conditions:
  - 100% thermal accommodation
  - 100% diffuse surface reaction
  - Temperature of all surfaces = 373 K

- Output:
  - rotational temperature, density and pressure

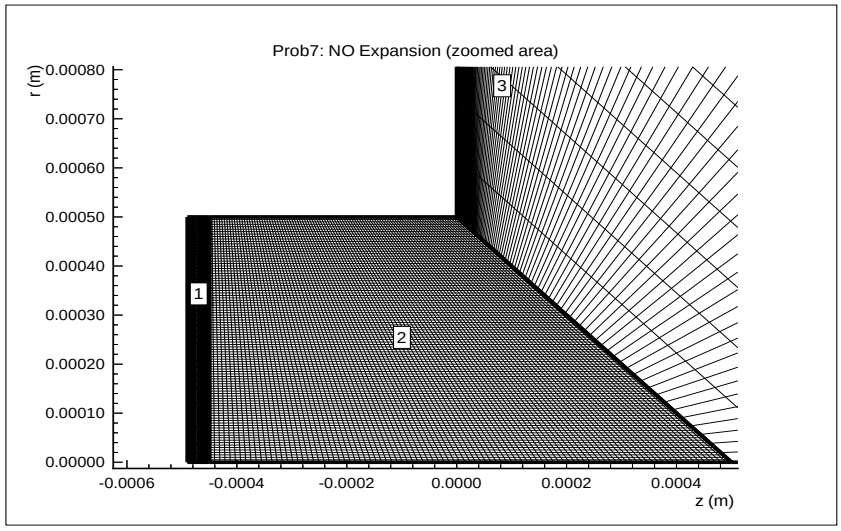
- Reference:

Bartel, T. J. & Justiz, C. R., "DSMC Simulation of Ionized Rarified Flows," AIAA 93-3095, AIAA, 24th AIAA Fluids Dynamics Conference, Orlando, FL, 1993.

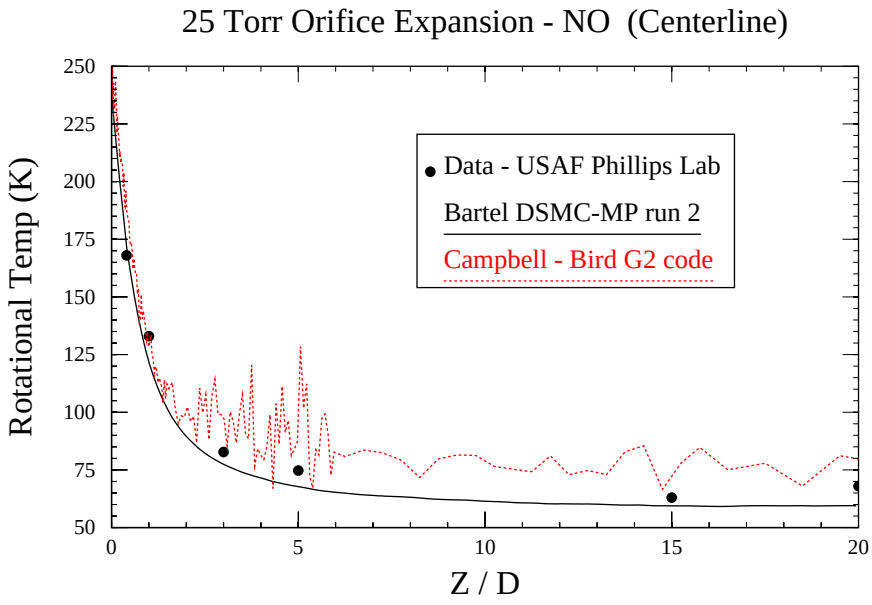
grid:

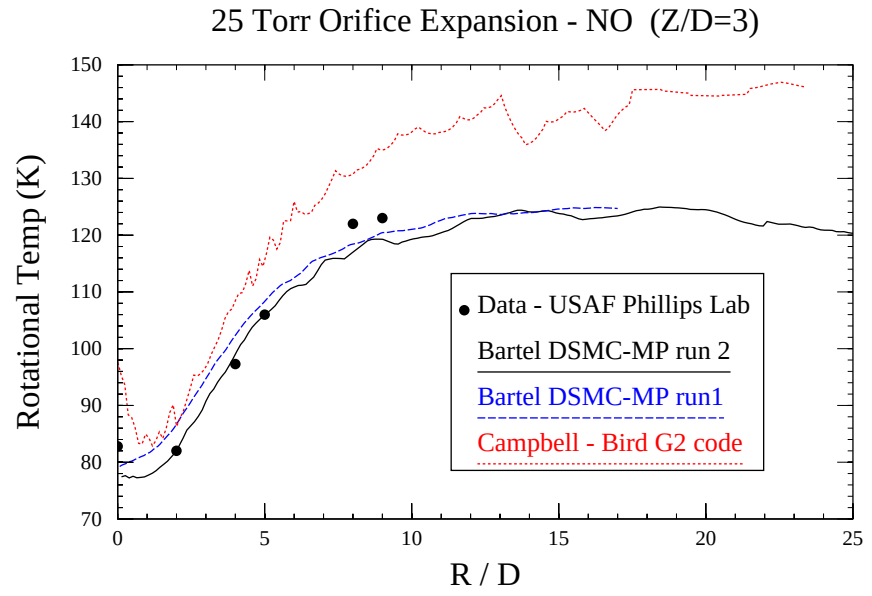


Zoomed area at gas inlet:



Comparisons to Data and Bird's G2 DSMC Code





TempleGraph 2.5, Origin: tjbarte@sass001 - Thu Jun 17 12:05:12 1993 (data file was DSMC-PV25T-XD3)

input file:

```
*-----------------------------------------------------------------------
*   asterick in column 1 indicates comment card
*-----------------------------------------------------------------------
  pulsed valve-25T- NO diffuse
*
*
*-----------------------------------------------------------------------
*
control              1      -1 -- plot grid only;
*                            1 -- initialization & plot file
*
type                 1              0/1 for X-Y or Z-R flow
*
cell weight          -4
expansion radius wt   0.0005
*
read general grid
*-----------------------------------------------------------------
*                   Region Definition
*-----------------------------------------------------------------
    4           number of regions (must be .le. 30)
    19           number of global points (must be .le.120)
*--------------------------------------
*     Global corner pt. coordinates
*  Pt.        z (m)          r(m)
*--------------------------------------
   1      -0.00045      0.0
   2      -0.00045      0.0005
*  3       0.0          0.0
   3       0.0005       0.00
   4       0.0          0.0005
   5       0.0          0.0050
   6       0.005        0.005
   7       0.005        0.00
   8       0.01         0.005
   9       0.025        0.00
  10       0.0          0.025
  11       0.01         0.01
  12       0.01         0.0005
  13       0.005        0.0005
  14      -0.00049      0.0
  15      -0.00049      0.0005
  16       0.002        0.00
  17       0.00         0.002
  18       0.015        0.03
  19       0.03         0.02
*
*=======================================================================
region    1  <------  Inputs specific to this region follow
*=======================================================================
```

```
grid
  14            global points coinciding w/ region corner points 1 - 4, resp.
  15
   2
   1
  30            number of cells along sides 1 and 3
  50            number of cells along sides 2 and 4
   0           sides 1 and 3 curvature:     0/1 for straight line/circular arc
   0           sides 1 and 3 cell spacing:
   3  1.03  50.  sides 2 and 4 cell spacing:
   1           boundary type code for sides 1 - 4, resp.
   5
  31
   7
   1           number of cells for which B.C.'s need to be  read
*-------------------------------------------------------------------------
*  Side  Cell1  Cell2  elem/cell    Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
   2    1     60       1        0.000        373.       0.          0.
*-------------------------------------------------------------------------
*-------------------------------------------------------------------------
*                Region interface/matching
*   Reg. side   reg. sides       Adj. side  Adj. reg.
*-------------------------------------------------------------------------
*-------------------------------------------------------------------------
      1         0
      2         0
      3         0
      4         1        2    2
*=========================================================================
region   2 <------  Inputs specific to this region follow
*=========================================================================
grid
   1            global points
   2
   4
   3
 100             number of cells along sides 1 and 3
 100             number of cells along sides 2 and 4
   0           sides 1 and 3 curvature: 0/1
   0           sides 1 and 3 cell spacing:
   0           sides 2 and 4 cell spacing:
   1           boundary type code for sides 1 - 4, resp.
   7
   5
   7
   1           number of cells for which B.C.'s need to be  read
*-------------------------------------------------------------------------
*  Side  Cell1  Cell2  elem/cell    Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
   3    1     100     1         0.000        373.       0.          0.
```

```
*---------------------------------------------------------------------
*---------------------------------------------------------------------
*                Region interface/matching
*   Reg. side   reg. sides       Adj. side  Adj. reg.
*---------------------------------------------------------------------
*---------------------------------------------------------------------
       1         0
       2         1         4    1
       3         0
       4         1         1    3
*=====================================================================
region    3   x <------  Inputs specific to this region follow
*=====================================================================
grid
   4              global points
  10
   9
   3
 100               number of cells along sides 1 and 3
 200               number of cells along sides 2 and 4
   0              sides 1 and 3 curvature: 0/1 for straight line/circular arc
   2  1.04  100.   sides 1 and 3 cell spacing:
   0              sides 2 and 4 cell spacing:
   7              boundary type code for sides 1 - 4, resp.
   5
   7
   1
   1              number of cells for which B.C.'s need to be  read
*---------------------------------------------------------------------
*   Side  Cell1  Cell2  elem/cell   Spec. refl.   Temp. K    Material#    Value
*---------------------------------------------------------------------
    2     1    200     1          0.000         373.       0.0          0.0
*---------------------------------------------------------------------
*---------------------------------------------------------------------
*                Region interface/matching data
*   Reg. side   reg. sides       Adj. side  Adj. reg.
*---------------------------------------------------------------------
*---------------------------------------------------------------------
       1         1              4          2
       2         0
       3         1              1          4
       4         0
*=====================================================================
region    4   x <------  Inputs specific to this region follow
*=====================================================================
grid
  10              global points
  18
  19
   9
  60              number of cells along sides 1 and 3
```

```
  40             number of cells along sides 2 and 4
   0             sides 1 and 3 curvature: 0/1 for straight line/circular arc
   0             sides 1 and 3 cell spacing:
   2  1.02   10.   sides 2 and 4 cell spacing:
   7             boundary type code for sides 1 - 4, resp.
   11
   11
   11
   0             number of cells for which B.C.'s need to be  read
*-------------------------------------------------------------------------
*   Side  Cell1  Cell2  elem/cell   Spec. refl.   Temp. K    Material#    Value
*-------------------------------------------------------------------------
*-------------------------------------------------------------------------
*-------------------------------------------------------------------------
*                  Region interface/matching data
*    Reg. side   reg. sides       Adj. side  Adj. reg.
*-------------------------------------------------------------------------
*-------------------------------------------------------------------------
       1         1             3          3
       2         0
       3         0
       4         0
*-------------------------------------------------------------------------
END               END OF EXPERT INPUT FILE
*-------------------------------------------------------------------------
```

inlet file:

```
*   freestream inlet condition for the ICF sphere
*
*      Xe species
*
1 number of tables
*
0   -----  flag to specify freestream conditions
3.216e20   400.    0.0     1500.   1500.   1500.    1.
*
```

species file:

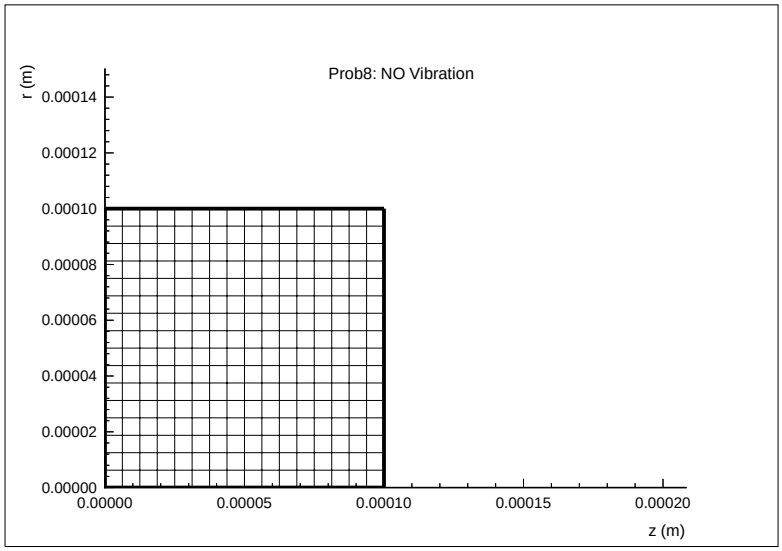
```
*****************************************
*      species data file            *
*****************************************
1          number of species
*
3          internal structure of most complex molecule:
*          3-monatomic, 4-rotation, 5-rotat. + vibrat.
*
0          # of chemical reactions
*
*-------------------------------------------------------------------------------------------------------------------
* ID
* Mwt     Mol. mass    Diam.   #Rot.Deg.     Rot.Rel.  # Vib. Deg.  Vib. Rel. Vib.Temp. specie wt. charge
omega   tref   alpha
*          (kg)      (m)     Freedom     Coll. #    Freedom     Coll. #     (K)
*-------------------------------------------------------------------------------------------------------------------
  Xe
  131.229  2.18e-25  5.74e-10      0.         5.         0.          0.         0.       1.0      0.0      .85    300.     1.
*
END
```

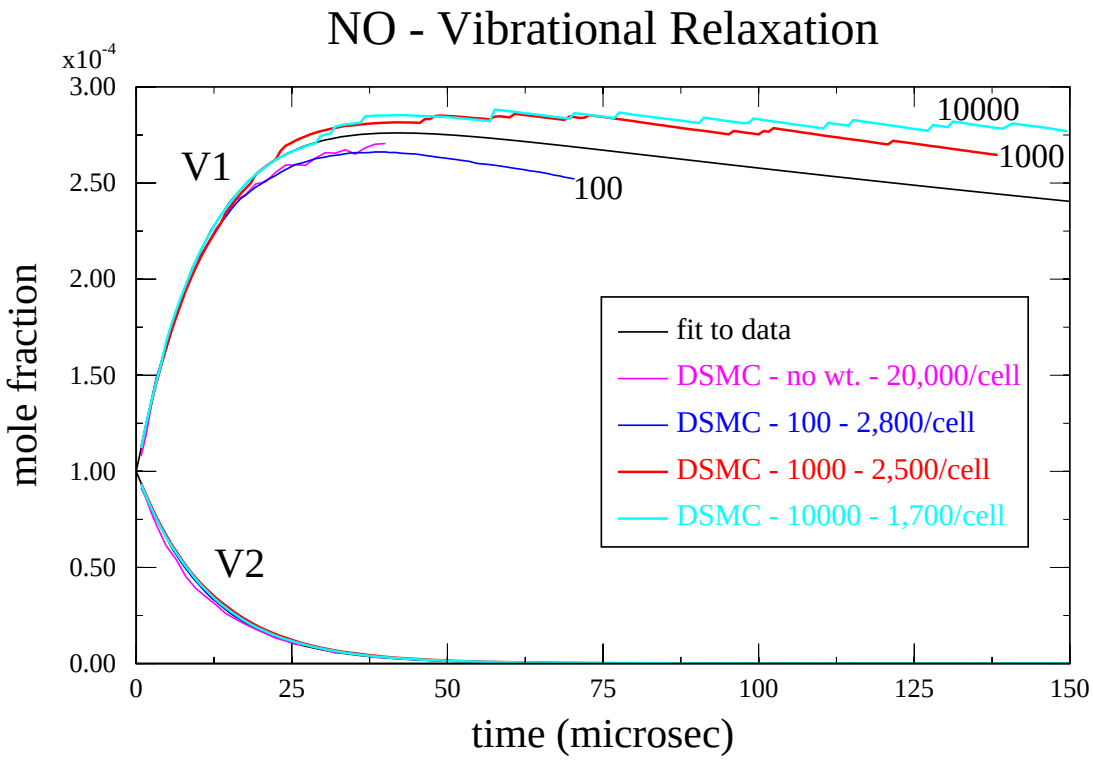
13.10 NO Vibrational Relaxation (Time Dependent)

This problem is a transient simulation of the vibrational relaxation of NO where states V0, V1, and V2 are modelled using a 6 reate equation model based on USAF Phillips Lab data. The simulation startes with a small amount (0.0001 mole fraction) of NO excited to V2 and V1 in a domain of V0. This simulations illustrates the trace species model in Icarus and the procedure to perform a transient simulation.
- Input Gases: NO

- Surface Boundary Conditions:
    - 100% thermal accommodation
    - 100% specular surface reaction
    - Temperature of all surfaces = 300 K

- Gas Phase Chemistry:
    6 gas phase reactions (refer to chemistry file)
- Output:
    - pressure, velocity, temperature and species distribution
    - portray species weighting model
    - time accurate mole fractions





input file:

```
------------------------------------------------------------------------
*   asterick in column 1 indicates comment card
*-----------------------------------------------------------------------
 1 Region NO vib. relaxation 3 levels
*
*-----------------------------------------------------------------------
*
*
control    1      -1 -- plot grid only;
*                  1 -- initialization & plot file
*
type       0              0/1 for X-Y or Z-R flow
*
read general grid
*-----------------------------------------------------------------------
*                    Region Definition
*-----------------------------------------------------------------------
     1           number of regions (must be .le. 30)
     4           number of global points (must be .le.120)
*--------------------------------------
*     Global corner pt. coordinates
*  Pt.        z (m)          r(m)
*--------------------------------------
```

```
   1       0.000         0.000
   2       0.000         1.0e-04
   3       1.0e-04       1.0e-04
   4       1.0e-04       0.000
*-------------------------------------------------------------------
*               Individual Region Definitions Follow
*              --REGIONS NUMBERS MUST BE SEQUENTIAL--
*-------------------------------------------------------------------
*===================================================================
region    1  <------  Inputs specific to this region follow
*===================================================================
grid
   1           global points coinciding w/ region corner points 1 - 4, resp.
   2
   3
   4
  16           number of cells along sides 1 and 3
  16           number of cells along sides 2 and 4
   0           sides 1 and 3 curvature:     0/1 for straight line/circular arc
   0           sides 1 and 3 cell spacing:
   0           sides 2 and 4 cell spacing:
   5           boundary type code for sides 1 - 4, resp.
   5
   5
   5
   4           number of bc entries
*-------------------------------------------------------------------
*   Side  Cell  Cell2  elem/cell   Spec. refl.    Temp. K    Material #   Value
*-------------------------------------------------------------------
    1    1    16    1          1.000        300.         0          0.
    2    1    16    1          1.000        300.         0          0.
    3    1    16    1          1.000        300.         0          0.
    4    1    16    1          1.000        300.         0          0.
*-------------------------------------------------------------------
*-------------------------------------------------------------------
*                 Region interface/matching
*    Reg. side   reg. sides       Adj. side  Adj. reg.
*-------------------------------------------------------------------
*-------------------------------------------------------------------
        1          0
        2          0
        3          0
        4          0
*-------------------------------------------------------------------
END               END OF EXPERT INPUT FILE
*-------------------------------------------------------------------
```

inlet file:

```
*
*   freestream inlet condition for NO relaxation
*
*     NO:  V0    V1    V2
*
1 number of tables
*
0   -----  flag to specify freestream conditions
 3.296e22    0.    0.0     293.   93.   293.   0.9998    0.0001   0.0001
*
```

species file:

```
****************************************
*       species data file              *
****************************************
3           number of species
*
4          internal structure of most complex molecule:
*           3-monatomic, 4-rotation, 5-rotat. + vibrat.
*
6           # of chemical reactions
*
*-------------------------------------------------------------------------------------------------------------
*  ID
*  Mwt      Mol. mass    Diam.    #Rot.Deg.      Rot.Rel.   # Vib. Deg.   Vib. Rel. Vib.Temp. specie wt. charge
omega   tref   alpha
*           (kg)       (m)     Freedom      Coll. #    Freedom      Coll. #     (K)
*-------------------------------------------------------------------------------------------------------------
*
*    this fit is for low temperature NO states;
v0
  30.0061  4.98E-26  4.26E-10      2.         1.         1.              1       0.     1.0         0.      0.9   300.     1.0
v1
  30.0061  4.98E-26  4.26E-10      2.         1.         1.              1.      0.    0.001        0.      0.9    300.    1.0
v2
  30.0061  4.98E-26  4.26E-10      2.         1.         1.              1.      0.    0.001        0.      0.9    300.    1.0
*
END
```

chemistry file:

```
*-----------------------------------------------------------------------
*  This input file contains the data characterizing the chemical reactions.
*
*-----------------------------------------------------------------------
* NO vibrational set 3 levels
V2 + V0 --> V1 + V1
*
0  3    1    1    1    2     2
```

```
0.          5.559E-22     1.706E-19     0.5        -5.559E-22
*
V1 + V0 --> V2 + V0
*
0  2    1    1    1    3    1
0.          3.669E-20     8.885E-21     0.5        -3.669E-20
*
V0 + VO --> V1 + V0
*
0  1    1    1    1    2     1
0.          3.725E-20     4.442E-21     0.5        -3.725E-20
*
V1 + V1 --> V2 + V0
*
0  2    2    1    1    3     1
0.          0.00          1.706E-19     0.5         5.559E-22
*
V2 + V0 --> V1 + V0
*
0  3    1    1    1    2     1
0.          0.00          8.885E-21     0.5         3.669E-20
*
V1 + V0 --> V0 + V0
*
0  2    1    1    1    1     1
0.          0.00          4.442E-21     0.5         3.725E-20
*
*  third body probabilities now follow
*
0
```

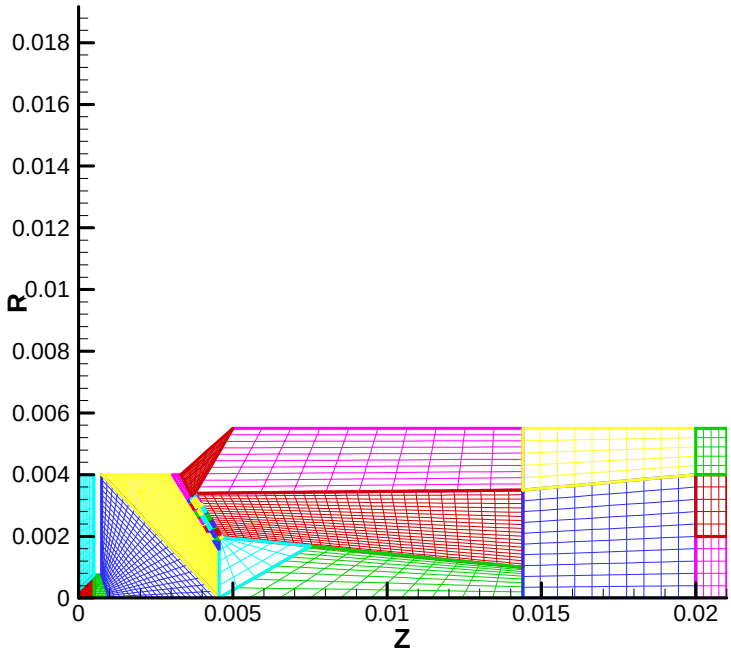
Icarus input file:

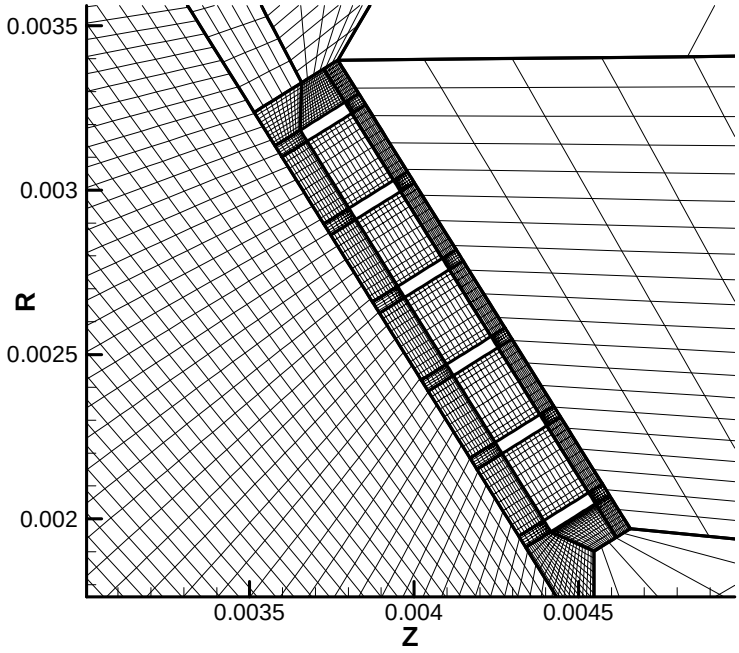
```
# Test file for VIb -- 1000

log file            dsmc.log

output screen       50

zero flag           50

random seed         3847


read def            1.0 dsmc.def

adapt flag           20000 0.25
time factor         0.002

output special      400
run                 100000 0
```

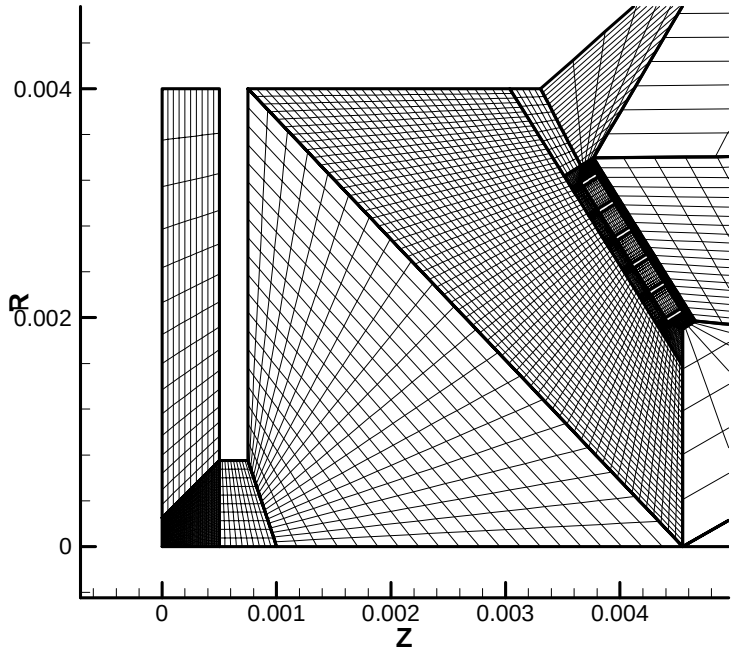
13.11 Ion Accelerator

This sample case has been included to demonstrate various input options for a complex chemically reacting plasma simulation. However, this grid was generated in the early portion of the project and later grids were more efficient and easier to modify. The problem is axisymmetric with an ion source located near the centerline on the left side of the grid: ions and neutrals are injected here. The fine details of the ion generation are beyond the scope of physics in Icarus. The plume expands into the vacuum until it reaches the screen region of the ion extractor/accelerator. Here, the electrons are extracted to the grid and a large potential is applied to accelerate the ions to a target. One should compare the gridding around the screen region in this problem with that in problem 13.5. Problem 13.5 was generated using the multiple connected region capability of Icarus to drastically reduce the number of regions in the domain and to greatly simplify the modification process.

The input files will not be reproduced here; they are available with the electronic form of this manual. This problem consists of 49 regions; regions 1-5 are defined as ambipolar and with a Poisson solver used to determine the electro-static fields for the remainder. Ions and neutrals are injected in the ambipolar region and the expansion due both to the simple half-spherical expansion and the ambipolar fields. When the ions enter the upstream region before the screen, 'heavy' electrons are injected as a rate to maintain quasi-neutrality in the initial cell. Now a Poisson solver is used to determine the electro-static fields. A 'heavy' electron is defined as simply 1000 times the mass of an electron (a pseudo-negative ion). The approximation gives up the accurate simulation of the sheaths at the screen for an 20 - 50 time larger time step. Secondary electrons in the acceleration region are 'real' electrons with the classical electron mass.




0.0035
0.003
0.0025
0.002
R
0.0035
0.004
0.0045
Z


0.004
0.002
0
R
0
0.001
0.002
0.003
0.004
Z

14.0 Distribution

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1	MS 0841	9100	T.C.Bickel
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1	MS 0826	9113	W. L. Hermina
1	MS 0826	9113	C.C.Wong
1	MS 0824	9115	J.L.Payne
1	MS 0824	9115	C. Roy
1	MS 0836	9117	M.A.Gallis
1	MS 0321	9200	W. J. Camp
1	MS 0310	9230	P. Yarrington
1	MS 0820	9232	P.F.Chavez
25	MS 0820	9232	T.J.Bartel
1	MS 0316	9233	R.C.Schmidt
1	MS 1111	9209	S.J.Plimpton
1	MS 0828	9132	S.N.Burchett
1	MS 1423	1118	M.Riley
1	MS 1423	1118	P.Miller
1	MS 1423	1118	J.Woodworth
1	MS 0521	2502	F.M.Bacon
1	MS 0516	2564	G.Laughlin
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